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Polyatomic Molecules With Internal Rotation

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MICROWAVE SPECTRAL TABLES

Volume III. Polyatomic Molecules With Internal Rotation

Paul F. Wacker, Marian S. Cord, Donald G. Burkhard,
Jean D. Petersen, and Raymond F. Kukol

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U.S.

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Microwave Spectral Tables

Volume III. Polyatomic Molecules With Internal Rotation

Paul F. Wacker, Marian S. Cord, Donald G. Burkhard,

Jean D. Petersen, and Raymond F. Kukol

Measured frequencies, assigned molecular species, and assigned quantum numbers are given for about 9,000 spectral lines of polyatomic molecules with internal rotation observed by coherent radiation techniques. Molecular data, such as rotational constants, dipole moments, and various coupling constants, determined by such techniques, are also tabulated. References are given for all included data.

Key Words: Microwave spectra, molecular spectra, spectral lines, rotational constant, quadrupole coupling constants, internal rotation, hindered rotation, centrifugal distortion constant, barrier height, dipole moment, polyatomic molecules, coherent radiation technique.

1. Introduction

This volume contains data on the microwave spectra of 94 polyatomic molecules capable of exhibiting internal rotation, based upon a search of the literature up to July, 1962, but including some information of later dates. In most cases some effects of internal rotation have been observed. In others it has not actually been observed but its existence can be inferred from structural information. These are molecules whose atoms can be arranged in groups in such a way that the groups are capable of rotating separately about common axes. This rotation is hindered by a potential. In the case that the chemical bond between the nearest atoms in two adjacent groups is a single one, it is supposed that the potential is small enough to permit observations of internal rotation effects, and such molecules are contained in this volume even if the internal rotation has not been observed. However, when the bonds are of higher order, the barrier to rotation is so high that torsional effects are most conveniently treated with techniques ordinarily used for vibration.

The theory of microwave spectra of molecules with internal rotation is briefly discussed by Townes and Schawlow[1] and in more detail by Lin and Swalen.[2] The following qualitative discussion, which is intended for readers not familiar with the field, is limited to molecules with two rotatable groups and therefore to a single internal rotation.

The hindering potential can be expressed, by means of a Fourier series, as a function of the difference α between the angular displacements of the two groups about a convenient common axis. If each group has a plane of symmetry containing the common axis, α may be defined so that no sine term occurs in the series. Further, if either group has axial symmetry, only terms in $n\alpha$ (where n is an integer) and its harmonics appear. Moreover, of the non-constant terms of the series, only the leading term is ordinarily considered; in most cases, agreement between theory and the available experimental data is so good that more laborious analysis is not considered justifiable. Then with this approximation the potential may be written as

$$V=\frac{V_n}{2}(1-\cos n\alpha), \qquad (1)$$

where n is an integer which depends upon the symmetry of the molecule. The barrier height, V (V_n in the preceding approximation), is a principal parameter to be determined by analysis of the spectra.

[1] C. H. Townes and A. L. Schawlow, Microwave Spectroscopy, McGraw Hill, N.Y. (1955).

[2] C. C. Lin and J. D. Swalen, Rev. Mod. Phys. **31**, 841 (1959).

The presence of internal motions greatly complicates the spectra. Therefore, it is not surprising that the molecules which have been studied are chiefly those where the situation is somewhat simplified by molecular symmetry. The principal theoretical treatments assume that at least one of the internally rotating portions has at least a three-fold axis of symmetry, i.e., that rotation of the group through the angle $2\pi/p$, where p is at least 3, yields a configuration which is indistinguishable from the original. The commonly encountered methyl group, as well as every symmetrically-substituted methyl group, has a three-fold axis. This portion is commonly referred to as the "top". If the first group has a p-fold axis and the second has a q-fold axis, the integer n is the least common multiple of p and q. Thus, n equals 3 if each rotatable group is a methyl group or a symmetrically substituted methyl group, or if one has three-fold symmetry and the other has no axis of symmetry.

Associated with the internal motion is a torsional quantum number v. If v is sufficiently low and if the barrier height V_n is sufficiently high that the kinetic energy of torsional motion is small compared to V_n, the internal motion can be considered that of torsional oscillation. However, the torsional levels may be split by quantum mechanical tunneling between the n equivalent relative orientations; this process is the angular analog of the well-known inversion of ammonia. In the opposite extreme, in which the internal motion is a free rotation, the levels are again split, although the details are different.[3] In either case, there are n states for each value of v, although there may be some degeneracies among these states. In the most frequently studied case, for $n = 3$, each rotational level is split into a single level of group-theoretical species A and a doubly-degenerate level of species E. For each given value of v, the A levels give rise to a spectrum which, to a first approximation, is of the same form as the spectrum of a rigid rotor, except that the rotational constants are functions of v. Transitions between A and E levels are forbidden since the dipole moment cannot be a function of α. In some cases the spectrum due to the E levels may resemble that of a rigid rotor and in other cases it may not, depending upon the barrier height and the asymmetry of the molecule. The separation between pairs of A and E levels is a measure of the barrier height and, therefore, is of prime interest. The spectra due respectively to the A and E levels are usually distinguishable experimentally by the Stark effect. The A spectrum, as with rigid asymmetric rotors, exhibits a quadratic effect, while the E spectrum often gives rise to a much larger Stark effect, frequently of a linear or quasi-linear character. The nature of the hyperfine pattern also often can be used to distinguish between the two types of spectra.

Two mathematical descriptions of these molecules have been widely used. One of these is called the Principal Axis Method (PAM). In this the internal motion is referred to the set of axes which makes the off-diagonal products of inertia of the molecule as a whole equal to zero. It is fixed to one of the two groups, which is referred to as the "frame." If one of the two groups does not have three-fold or higher axial symmetry, it is the one chosen as the frame because then the moments and products of inertia are independent of the angle α, and if the principal axes have been selected to make the products of inertia zero for one value of α, they remain zero for all others. In this system the quantities which are of fundamental interest are: (1) the principal moments of inertia and their associated rotational constants A, B, and C, where $A \geqq B \geqq C$; (2) the moment of inertia I_α of the top with respect to the axis of internal rotation; and (3) the direction cosines (λ) of the axis of internal rotation with respect to the principal axes.

The other is the Internal Axis Method (IAM) in which the axis of internal rotation is chosen as one of the axes used to express the rotational energy of the molecule. Here the following quantities are of fundamental interest: (1) moments of inertia and rotational constants with respect to the principal axes; (2) direction cosines of the internal axes relative to the principal axes; (3) moments and products of inertia of the whole molecule with respect to the internal axes; and (4) the moments of inertia of the two parts of the molecule with respect to the internal axis.

In the Hamiltonian, the kinetic energy may be expressed in three parts: (1) that due to the rotation of the molecule; (2) that due to the internal rotation: and (3) that due to interaction between (1) and (2). In the PAM, both the overall rotation and the internal rotation are simply expressed, and the interaction is treated as a perturbation; if the interaction is readily handled, this procedure is quite convenient. In the IAM, the interaction terms are ordinarily considerably smaller than in the PAM, permitting a relatively simple perturbation treatment. The chief disadvantage of the IAM is that the failure to use principal axes complicates the Hamiltonian by introducing terms containing products of inertia. To provide further simplification, it may be necessary to introduce transformations to additional coordinate systems, each

[3] This splitting occurs even for zero barrier.

requiring the definition of additional quantities. Further details, as well as the method of translating between PAM and IAM data, can be found in the review paper by Lin and Swalen.[2] Such additional symbols as are required for the purposes of these tables will be defined later.

In these tables an attempt has been made to list quantities obtained directly from experiment and to utilize structural information or hypotheses to the very minimum possible, since the latter are subject to change and, frequently, to controversy. In cases where analysis requires some structural information, the results from the authors' analyses have been given in order to minimize the uncertainty arising from structural information.

There do exist some nonuniformities of style as some authors have employed uncommon notations, and it has been found desirable to have the results remain in their notation.

To minimize typographical errors, the data for the tables were punched on cards, converted to magnetic tape, listed, and then thoroughly compared with the original documents. No manual typesetting was used for the tables proper or their headings. Instead, the automatic photocomposition equipment of the Government Printing Office was controlled by tape prepared from the aforementioned data tape by means of computer programs. The control tape commands necessarily were detailed and included those for the chemical formulas, superscripts, subscripts, vertical and horizontal lines, spacings, and all characters, allowing for the variable character widths.

The Authors gratefully acknowledge invaluable assistance: in reviewing, from Yardley Beers, Robert Wallis and Jack Ross; in programming, from Matthew S. Lojko, and Jean Tucker; in checking, from Abiodun Afonga, Rudolph Haas, Emmett MacKenzie, Nancy Mills, and Marion Hinchman. The volume could not have been finished for publication without their contributions. Thanks are also due the many scientists in the field of Microwave Spectroscopy who so graciously replied to requests for information.

2. Explanation of Tables

Data for these Microwave Spectral Tables have been compiled from a review of articles found in all internationally recognized journals as well as private communications regarding unpublished work. Generally speaking, date and accuracy of data measurement were the criteria by which any required selection was made. An explanation of the format and contents of the tables follows.

The first line of data contains an identification number and the Chemical Abstracts name. The lines immediately following give alternate names, if any. The last line of the heading contains the empirical formula, the symmetry point groups, and (where possible) the "quasi-" structural formula. The first point group is for the molecule as a whole, assuming only one isotopic form of each element and the configuration believed to have the lowest potential energy. The parentheses contain the point group of each independently rotatable portion (with associated bonds). For a straight-chain molecule, the order is that of the structural formula. Molecules are indexed first according to empirical formula, as in Chemical Abstracts, then alphabetically by name. A numbering system has been established for identification of the molecules and their isotopic species for convenience in programming and referencing. Each molecule was given a number ending in zero in order of its occurrence on the list. Its species have been numbered consecutively from that point, skipping the next zero when the number of isotopic species exceeds nine. Every species is given for which any molecular constants or spectral lines from microwave sources have been reported through June 1962. In the formulas for the species, mass numbers have been placed as superscripts to the right of the atomic symbols. Hydrogen is the one exception—for the normal mass of 1 the superscript is omitted and for deuterium (H^2) the symbol D is used.

In the second column of the molecular constant table, the overall symmetry point group (Pt. Gp.) has been given for each isotopic species of the molecule as the analysis permits. Some consideration of structural information was necessarily a part of these assignments.

Most of the rotational constants tabulated have been derived from microwave sources, and this is indicated by the M occurring after the values. In a few instances, other experimental sources have been designated by the code letter N for near infrared measurements. Use of symmetry has been made in reporting rotational constants. If, for example, the axis of symmetry of a symmetric top is known to be the axis of least moment of inertia,

then the constants B and C are equal and are so recorded. Every moment of inertia has been converted to the corresponding constant A, B, or C (in megahertz) by multiplication with the appropriate conversion factor. These factors are given later.

Centrifugal distortion effects are more important in the microwave spectra of asymmetric rotors than in the case of symmetric tops and more important with light molecules than with heavy molecules. The constants D_J and D_{JK} are dependent upon the rotational constants and the vibrational force constants. Although both D_J and D_{JK} are small in comparison with the values of the rotational constants, they serve to complicate the relationship between the other parameters and the frequency ν. Townes and Schawlow [4] state that D_J is always positive, but D_{JK} is positive or negative depending upon the type of molecule.

The asymmetry parameter

$$\kappa=\frac{2B-A-C}{A-C}$$

is a measure of the variation from the symmetric top. For a prolate top, $\kappa=-1$ and for an oblate top, $\kappa=+1$. Hence κ ranges between these two values. In cases where the original papers have used other parameters, these have been converted to κ values. Formulas which were used for these conversions are as follows:

$$\kappa=2\delta-1=\frac{3b_p+1}{b_p-1}=\frac{1+3b_0}{1-b_0};$$

b_p and b_0 refer to prolate and oblate symmetric tops respectively.

With planar molecules the inertial defect, $\Delta=I_c-I_a-I_b$, is frequently of interest. Classically, for a rigid molecule, this is zero, but in actuality it is nonzero because of the existence of zero point vibrations.

In many instances, the total dipole moment μ was found in the literature, but it had not been resolved into a, b, and c components. Symmetric top molecules have two equal principal moments of inertia, denoted by I_b. The dipole moment of such molecules lies along the principal axis with the unequal moment of inertia. Some of the original papers did not specify whether this moment of inertia was smaller or larger than the two others and, therefore, did not indicate whether this third axis should be labelled a or c. An effort was made to resolve this question by making use of available structural information to calculate the moment of inertia with respect to the symmetry axis according to the formula

$$I_{sym}=n\ m\ l^2\ \sin^2\phi,$$

where n is here the number of equivalent off-axis atoms or groups, m is the mass of the off-axis atom or group, l is its distance along the bond to the axis, and ϕ is the angle between the bond and the symmetry axis. Where $n=3$ and θ is the angle between the bonds from the axis to a pair of equivalent off-axis atoms, the formula becomes

$$I_{sym}=2\ m\ l^2\ (1-\cos\theta).$$

(Townes & Schawlow, p. 53)

Using the convention $I_a \leqq I_b \leqq I_c$, if the computed value was smaller than the given I_b then the figure axis was a, if greater than I_b then the figure axis was c. A symbol M follows the value if the dipole moment was measured by microwave techniques, usually the Stark effect. In the case of asymmetric molecules, if the components of the dipole moment were not specified, the reported dipole moment was entered under the component which was adjudged the major one (according to transitions assigned to frequency lines, or, if these were lacking, according to structural information available). In addition, the letter u designates the unknown (but possible) second or third component. The code letter T is used after the dipole moment entry if it was not obtained by microwave techniques unless the moments were known to be obtained from the Debye equation with temperature-variation data for the molar polarization of the gas or liquid. In these cases designations G or L are used. Dipole moment components known to be zero by virtue of established symmetries are indicated by an X after the data (for example, a component perpendicular to the plane of symmetry, or one in a plane perpendicular to the axis of symmetry, would always be zero). Effects of isotopic substitution on the symmetry of the molecule have been taken into account.

Quadrupole coupling constants, eQq, obtained from hyperfine structure measurements are reported as found in the literature. These relate to the energy of interaction between the molecule and the nuclear quadrupole moment. In some cases the authors have reported these as referred to the principal axes or with reference to a particular bond, and if so, they are recorded thus. Potential barrier heights are designated by V. Integer subscripts

[4] Townes and Schawlow, Microwave Spectroscopy, McGraw-Hill Book Co., pp. 77–79, 105–109 (1955).

are used to designate components corresponding to individual terms in the Fourier series expressing the potential. The number n is related to the symmetry of the molecule as described in the introduction. In a few cases the reduced moment of inertia (I_{red}) is given. Microwave values of the torsional frequencies (which also provide measures of the barriers) are given in cm^{-1}. To facilitate later description of transitions involving excited vibrational states, each vibrational mode excited in any observed microwave transition is assigned a letter subscript and is identified by the frequency ω in cm^{-1} and the degeneracy d.

The table of reported spectral lines for each molecule starts on the page with or following the molecular constant table. Lines for each isotopic molecular species are arranged in the following pattern: ascending order of rotational quantum numbers according to

$$(1)J', (2)\ J, (3)\ K'_{-1}, (4)\ K_{-1}, (5)\ K'_{+1}, (6)\ K_{+1},$$

then in ascending magnitude of frequency. Immediately following the heading for the spectral lines the formula and identification number of the isotopic molecular species are printed. For asymmetric tops the rotational quantum numbers are arranged in the pattern

$$J', K'_{-1}, K'_{+1} \leftarrow J, K_{-1}, K_{+1},$$

where primes denote upper state. For prolate or oblate symmetric tops the arrangement is

$$J', K'_{-1} \leftarrow J, K_{-1} \text{ or } J', K'_{+1} \leftarrow J, K_{+1},$$

respectively; for linear molecules simply $J' \leftarrow J$. Unassigned lines are so indicated. Blanks occur where the identification was not complete. It should be recognized that unassigned lines may be due to impurities and may be spuriously associated with a particular molecule.

Also, it should be mentioned that, in a few $\Delta J = \pm 1$ transitions of very asymmetric molecules, it is difficult to ascertain which is the upper state even if quantum numbers have been assigned to both states. There is indication that some authors have not clearly stated the existence of this uncertainty or that they have been careless with their notation in this regard. In some instances clarification has been obtained, but in others this was not possible. In any event the quantum numbers on the left denote the state which is believed to be the upper state.

For the most part, unless there is reason to suppose otherwise, the ground vibrational state has been assumed where the specific state was not mentioned. For each transition corresponding to an excited vibrational state, the vibrational quantum number of each excited normal mode is given. These are identified by v_a, v_b, etc., the letter subscripts corresponding to the mode identifications introduced in the molecular constant table.

More than one format is used in the portion of the table dealing with internal rotation, since the appropriateness of format and notation varies with the number of rotating groups, the symmetry of the molecule, and the barrier heights. Insofar as was possible, the A and E state and n designation has been maintained. However, special cases have arisen where it was not possible to translate the notation given in the article into these terms. Attempts have been made to use the same notation found in the reference from which the material was taken and it is not our purpose to duplicate here detailed explanations of these special formats. The reader should consult the referenced literature for the author's explanation.

There is considerable nonuniformity in the listing of hyperfine components mainly because many times only a few of the rotational transitions of a given molecule may have their hyperfine splittings analyzed. If the hyperfine splitting is resolved, the individual lines are ordinarily reported separately in the present tables with the total angular momenta F′ and F of the upper and lower states, respectively. If the splitting is partially resolved, the assigned F values are given for the resolved lines. For large J values, the $\Delta F = \Delta J$ components are relatively strong and displaced very little from the frequency the line would have if there were no hyperfine splitting. If the hyperfine splitting is quite small (less than 5MHz), the frequency of the hypothetical line for zero quadrupole moment is commonly listed and shifts from these frequencies given in the tables of spectral lines or footnotes to them.

Efforts were made to determine from the author's statement, the accuracies to which spectral lines were measured, though in many cases, these were not well defined in the literature. References are indicated for all data, but wherever practicable footnotes have been given to obviate the necessity of referring to these. References are arranged in order of year of publication, then alphabetically according to first author and numbered consecutively. A few exceptions occur in the case of books and of articles which were not reviewed until after the numbering had been completed and a change in reference number would have necessitated extensive changes throughout the whole volume.

3. List of Symbols, Abbreviations, and Conversion Factors

Symbols and Abbreviations

The following symbols and abbreviations are listed in the order in which they may first occur in the tables.

Molecular Constant Table

:	Double bond.
⋮	Triple bond.
. . .	Extra (cyclic) bond between two atoms preceding these symbols.
a-	Asymmetric.
b	As a superscript to an atomic symbol, indicates isotope not stated.
c-	Cis structure.
g-	Gauche structure.
t-	Trans structure.
s-	Symmetric.
Pt. Gp.	Symmetry point group of the molecular species.
Id. No.	Identification number of the molecule or molecular isotopic species.
A, B, C	Rotation constants (MHz). $A \geqq B \geqq C$.
M	Microwave determination.
N	Near infrared determination.
D_J, D_{JK}, D_K	Centrifugal distortion constants (MHz).
κ	Ray's asymmetry parameter, $(2B-A-C)/(A-C)$.
Δ	Inertial defect (amu Å^2).
a, b, c	Principal axes corresponding to A, B, and C, respectively.
$\mu_{a,b,c}$	Components of the dipole moment along the principal axes (Debye).
D	Abbreviation for Debye units.
u	Value not known.
X	Value precisely zero due to symmetry.
V	Barrier height, $V_{max}-V_{min}$ (cal/mol).
Acc	Accuracy of any previous quantity.
I_{red}	Reduced moment of inertia (amu Å^2).
eQq	For a symmetric top, the electric quadrupole coupling constant along the symmetry axis (MHz).
$\omega_{a,b,\ldots}$	Vibrational frequencies of modes a, b, . . excited in observed microwave spectral lines (cm^{-1}).
d	Degeneracy of the preceding vibrational mode.
Ref.	Numbers are reference numbers as in the bibliography.
$eQq_{aa}, \ldots$ $\chi_{aa}, \ldots$	Electric quadrupole coupling constant along indicated principal axis (MHz).
V_n	Coefficient of cos $n\alpha$ in the Fourier series for the potential barrier function (cal/mol).
I_α	Moment of inertia of rotatable group (amu Å^2).
$I_{a,b,c}$	Moments of inertia of the whole molecule with respect to the indicated principal axes.

Spectral Line Table

$v_a; v_b; \ldots$	Quantum number of the vibrational mode identified as a, b, . . in the molecular constant table. The ℓ quantum number is given after a comma rather than as a superscript.
A, E, . .	Symmetry species of the internal rotor state.
n	Torsional quantum number.
$F_1', ., . F$	Total angular momentum quantum number. Primed values are for the upper state, unprimed values for the lower state. Those with subscript I include nuclear spin only for nucleus with largest eQq.

Conversion Factors

The following formulas were used to convert the literature values x to the values y of the tables. The respective units are given in parentheses. It should be pointed out that the conversion factor given here for amu-Å^2 to MHz is based on the atomic weight scale in which $C^{12}=12$. However, most data covered in these tables were based on the older scale in which $O^{16}=16$.

amu Å^2 to MHz: $$y(\text{MHz}) = \frac{(8.391420\times10^5)}{x(\text{amu Å}^2)(1.6604345)} = \frac{(5.0537497\times10^5)}{x(\text{amu Å}^2)}$$

cm^{-1} to MHz: $$y(\text{MHz}) = (2.997925\times10^4)\, x(\text{cm}^{-1})$$

gm-cm^2 to MHz: $$y(\text{MHz}) = \frac{(8.3914204\times10^5)}{x(\text{gm-cm}^2)}$$

cm^{-1} to cal/mol: $$y(\text{cal/mol}) = 2.859\, x(\text{cm}^{-1})$$

4. Tables of Microwave Spectra of Molecules

Listed According to Empirical Formula

F_2O_2 $C_2(C_s.C_s)$ FOOF

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$F_2^{19}O_2^{16}$	C_2	11	20 266.18 M	5 011.09 M	4 360.14 M			−.9182	
$F_2^{19}O^{16}O^{18}$	C_1	12	19 531.98 M	4 975.78 M	4 318.68 M			−.9136	
$F_2^{19}O_2^{18}$	C_2	13	18 859.19 M	4 938.34 M	4 279.31 M			−.9096	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_2	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
11	0. X	1.44 M	0. X		30000						

References:

ABC: 345 D_J: D_{JK}: κ: 345 Δ:

μ: 345 eQq: V: 345 I: ω:

Dioxygen Difluoride

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$F_2^{19}O_2^{16}$	11	1, 1, 1← 0, 0, 0	Excited	1					24 484.06	.1	345
		1, 1, 1← 0, 0, 0	Ground						24 626.32	.1	345
		1, 1, 1← 0, 0, 0	Ground	1					24 715.57	.1	345
		1, 1, 1← 0, 0, 0	Ground	2					24 804.00	.1	345
		1, 1, 0← 1, 0, 1	Excited	1					15 817.85	.1	345
		1, 1, 0← 1, 0, 1	Ground						15 906.04	.1	345
		1, 1, 0← 1, 0, 1	Ground	1					16 016.74	.1	345
		1, 1, 0← 1, 0, 1	Ground	2					16 127.52	.1	345
		1, 1, 0← 1, 0, 1	Ground	3					16 239.55	.1	345
		1, 1, 0← 1, 0, 1	Ground	4					16 353.	.5	345
		2, 1, 2← 1, 0, 1	Ground						33 346.88	.1	345
		2, 1, 2← 1, 0, 1	Ground	1					33 414.80	.1	345
		2, 1, 2← 1, 0, 1	Ground	2					33 480.62	.1	345
		2, 1, 2← 1, 0, 1	Ground	3					33 539.31	.1	345
		2, 1, 1← 2, 0, 2	Excited	1					16 491.51	.1	345
		2, 1, 1← 2, 0, 2	Ground						16 577.38	.1	345
		2, 1, 1← 2, 0, 2	Ground	1					16 700.24	.1	345
		2, 1, 1← 2, 0, 2	Ground	2					16 822.03	.1	345
		2, 1, 1← 2, 0, 2	Ground	3					16 944.86	.1	345
		2, 1, 2← 3, 0, 3	Ground						13 406.8	.5	345
		2, 2, 1← 3, 1, 2	Ground						16 690.0	.5	345
		3, 1, 2← 3, 0, 3	Excited	1					17 540.88	.1	345
		3, 1, 2← 3, 0, 3	Ground						17 622.05	.1	345
		3, 1, 2← 3, 0, 3	Ground	1					17 764.15	.1	345
		3, 1, 2← 3, 0, 3	Ground	2					17 903.30	.1	345

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$F_2^{19}O_2^{16}$	11	3, 1, 2← 3, 0, 3	Ground	3					18 042.39	.1	345
		3, 1, 2← 3, 0, 3	Ground	4					18 182.24	.1	345
		4, 0, 4← 3, 1, 3	Ground	2					23 314.70	.1	345
		4, 0, 4← 3, 1, 3	Excited	1					23 436.63	.1	345
		4, 0, 4← 3, 1, 3	Ground	1					23 443.76	.1	345
		4, 0, 4← 3, 1, 3	Ground						23 563.25	.1	345
		4, 1, 4← 3, 0, 3	Ground						49 860.8	.5	345
		4, 1, 4← 3, 0, 3	Ground	1					49 870.9	.5	345
		4, 1, 4← 3, 0, 3	Ground	2					49 880.2	.5	345
		4, 1, 3← 4, 0, 4	Ground						19 084.40	.1	345
		4, 1, 3← 4, 0, 4	Ground	1					19 253.5	.5	345
		4, 1, 3← 4, 0, 4	Ground	2					19 418.45	.1	345
		4, 1, 3← 4, 0, 4	Ground	3					19 581.70	.1	345
		5, 0, 5← 4, 1, 4	Ground	3					33 484.7	.5	345
		5, 0, 5← 4, 1, 4	Ground	2					33 625.6	.5	345
		5, 0, 5← 4, 1, 4	Excited	1					33 700.7	.5	345
		5, 0, 5← 4, 1, 4	Ground	1					33 765.25	.1	345
		5, 0, 5← 4, 1, 4	Ground						33 871.6	.5	345
		5, 1, 4← 5, 0, 5	Ground						21 019.40	.1	345
		5, 1, 4← 5, 0, 5	Ground	1					21 225.3	.5	345
		5, 1, 4← 5, 0, 5	Ground	2					21 424.8	.5	345
		5, 1, 4← 5, 0, 5	Ground	3					21 620.05	.1	345
		6, 1, 5← 6, 0, 6	Excited	1					23 433.29	.1	345
		6, 1, 5← 6, 0, 6	Ground						23 488.36	.1	345
		6, 1, 5← 6, 0, 6	Ground	1					23 743.20	.1	345
		6, 1, 5← 6, 0, 6	Ground	2					23 986.65	.1	345
		6, 1, 5← 6, 0, 6	Ground	3					24 224.09	.1	345
		7, 1, 6← 7, 0, 7	Ground						26 552.38	.1	345
		8, 1, 7← 8, 0, 8	Ground						30 258.95	.1	345
		9, 1, 8← 9, 0, 9	Ground						34 636.60	.1	345
$F_2^{19}O^{16}O^{18}$	12	1, 1, 1← 0, 0, 0	Ground						23 850.65	.1	345
		1, 1, 0← 1, 0, 1	Ground						15 213.30	.1	345
		1, 1, 0← 1, 0, 1	Ground	1					15 319.85	.1	345
		2, 1, 2← 1, 0, 1	Ground						32 488.1	.5	345
		2, 1, 1← 2, 0, 2	Ground						15 892.15	.1	345
		3, 1, 2← 3, 0, 3	Ground						16 950.37	.1	345
		3, 1, 2← 3, 0, 3	Ground	1					17 089.0	.5	345
		4, 0, 4← 3, 1, 3	Ground						23 951.57	.1	345
		5, 0, 5← 4, 1, 4	Ground						34 171.9	.5	345
$F_2^{19}O_2^{18}$	13	1, 1, 1← 0, 0, 0	Ground						23 138.5	.5	345
		1, 1, 0← 1, 0, 1	Ground						14 579.88	.1	345
		2, 1, 2← 1, 0, 1	Ground						31 697.0	.5	345
		2, 1, 1← 2, 0, 2	Ground						15 261.76	.1	345
		3, 1, 2← 3, 0, 3	Ground						16 327.46	.1	345
		5, 0, 5← 4, 1, 4	Ground						34 395.9	.5	345

F_4N_2 $C_2(C_s,C_s)$ F_2NNF_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$F_2^{19}N^{14}N^{14}F_2^{19}$	C_2	21	5 576.21 M	3 189.35 M	2 812.95 M			−.7276	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_2	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
21	0. X	0. X	0.26 M		>3000						

References:

ABC: 255 D_J: D_{JK}: κ: 255 Δ:

μ: 255 eQq: V: 255 I: ω:

Add. Ref.: 362

Torsional frequency = 100 to 150 cm^{-1}. Ref: 255.

Tetrafluorohydrazine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$F_2^{19}N^{14}N^{14}F_2^{19}$	21	2, 2, 0← 1, 1, 0	Ground						19 582.6	.3	255
		2, 2, 1← 1, 1, 1	Ground						19 917.9	.2	255
		3, 1, 2← 2, 0, 2	Ground						21 725.0	.2	255
		3, 2, 1← 2, 1, 1	Ground						25 370.14	.05	255
		3, 2, 2← 2, 1, 2	Ground						26 297.	1.	255
		3, 3, 0← 2, 2, 0	Ground						30 868.47	.05	255
		3, 3, 1← 2, 2, 1	Ground						30 906.52	.05	255
		4, 1, 3← 3, 0, 3	Ground						28 549.9	.3	255
		4, 2, 2← 3, 1, 2	Ground						31 187.4	.1	255
		4, 2, 3← 3, 1, 3	Ground						32 856.	1.	255
		9, 5, 4← 9, 4, 6	Ground						22 866.9	.3	255
		10, 5, 5←10, 4, 7	Ground						22 805.9	.3	255
		11, 5, 6←11, 4, 8	Ground						22 788.3	.3	255
		12, 5, 7←12, 4, 9	Ground						22 865.6	.3	255
		13, 5, 8←13, 4,10	Ground						23 110.0	.3	255
		14, 5, 9←14, 4,11	Ground						23 620.1	.3	255
		14, 6, 8←14, 5,10	Ground						27 526.5	.3	255
		15, 5,10←15, 4,12	Ground						24 512.5	.3	255
		15, 6, 9←15, 5,11	Ground						27 461.3	.3	255
		16, 6,10←16, 5,12	Ground						27 501.8	.3	255
		17, 6,11←17, 5,13	Ground						27 723.1	.3	255
		18, 6,12←18, 5,14	Ground						28 226.0	.3	255
		19, 6,13←19, 5,15	Ground						29 131.5	.3	255
		20, 6,14←20, 5,16	Ground						30 572.0	.3	255
		21, 6,15←21, 5,17	Ground						32 669.0	.3	255

HNO_3 $C_s(C_s,C_{2v})$ HNO_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$HN^{14}O_3^{16}$	C_s	31	13 011.15 M	12 099.93 M	6 260.60 M			.73003	.11467
$DN^{14}O_3^{16}$	C_s	32	12 970.71 M	11 312.82 M	6 034.86 M			.52192	.10710
$HN^{15}O_3^{16}$	C_s	33	13 012.35 M	12 096.97 M	6 260.09 M			.72886	.11467

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
31	1.99 M	0.83 M	0. X		9400						

References:

ABC: 304 D_J: D_{JK}: κ: 304 Δ: 304

μ: 304 eQq: V: 129 I: ω:

For species 31, the quadrupole coupling constants are: $eQq_{aa} = .93 \pm .05$ MHz, $eQq_{bb} = -.82 \pm .05$ MHz, and $eQq_{cc} = -.11 \pm .10$ MHz.
For species 32, the quadrupole coupling constants are: $eQq_{aa} = .82 \pm .05$ MHz, $eQq_{bb} = -.62 \pm .05$ MHz, and $eQq_{cc} = -.20 \pm .10$ MHz.
Ref: 304.

Nitric Acid Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$HN^{14}O_3^{16}$	31	1, 0, 1← 0, 0, 0	Ground			0		1	18 360.06		304
		1, 0, 1← 0, 0, 0	Ground			2		1	18 360.48		304
		1, 0, 1← 0, 0, 0	Ground			1		1	18 360.78		304
		1, 1, 1← 0, 0, 0	Ground			1		1	19 271.45		304
		1, 1, 1← 0, 0, 0	Ground			2		1	19 271.69		304
		1, 1, 1← 0, 0, 0	Ground			0		1	19 272.06		304
		2, 1, 2← 1, 0, 1	Ground						31 792.80		304
		2, 1, 2← 1, 1, 1	Ground			1		0	30 881.24		304
		2, 1, 2← 1, 1, 1	Ground			3		2	30 881.69		304
		2, 1, 2← 1, 1, 1	Ground			2		1	30 881.92		304
		2, 1, 1← 2, 0, 2	Ground						17 616.03		147
		2, 1, 1← 2, 1, 2	Ground						17 517.51		304
		3, 2, 1← 3, 1, 2	Ground						16 700.74		147
		3, 2, 1← 3, 2, 2	Ground						16 215.59		304
		3, 3, 1← 3, 1, 2	Ground						22 161.00		147
		3, 3, 0← 3, 2, 1	Ground						9 447.97		147
		3, 3, 1← 3, 2, 2	Ground						21 676.16		147
		4, 3, 1← 4, 3, 2	Ground						14 534.25		304
		5, 3, 2← 5, 3, 3	Ground						29 175.32		304
		5, 4, 1← 5, 4, 2	Ground						12 540.98		304
		6, 4, 2← 6, 4, 3	Ground						27 369.67		304
		6, 5, 1← 6, 5, 2	Ground						10 344.23		304
		7, 5, 2← 7, 5, 3	Ground						24 903.51		304
		7, 6, 1← 7, 6, 2	Ground						8 097.58		304
		8, 6, 2← 8, 6, 3	Ground						22 147.00		304
		9, 7, 2← 9, 7, 3	Ground						18 969.56		304
		10, 8, 2←10, 8, 3	Ground						15 628.19		304
		11, 9, 2←11, 9, 3	Ground						12 317.35		304
		12,10, 2←12,10, 3	Ground						9 245.56		304

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$DN^{14}O_3^{16}$	32	1, 0, 1← 0, 0, 0	Ground			0		1	17 347.27		304
		1, 0, 1← 0, 0, 0	Ground			2		1	17 347.64		304
		1, 0, 1← 0, 0, 0	Ground			1		1	17 347.89		304
		1, 1, 1← 0, 0, 0	Ground			1		1	19 005.40		304
		1, 1, 1← 0, 0, 0	Ground			2		1	19 005.61		304
		1, 1, 1← 0, 0, 0	Ground			0		1	19 005.89		304
		2, 1, 2← 1, 0, 1	Ground						31 075.40		304
		2, 1, 2← 1, 1, 1	Ground			1		0	29 417.40		304
		2, 1, 2← 1, 1, 1	Ground			2		1	29 417.40		304
		2, 1, 2← 1, 1, 1	Ground			3		2	29 417.40		304
		2, 1, 1← 2, 1, 2	Ground						15 832.83		304
		3, 1, 2← 3, 1, 3	Ground						29 138.41		304
		3, 2, 1← 3, 2, 2	Ground						13 579.09		304
		4, 2, 2← 4, 2, 3	Ground						27 215.84		304
		4, 3, 1← 4, 3, 2	Ground						10 807.99		304
		5, 3, 2← 5, 3, 3	Ground						24 229.63		304
		5, 4, 1← 5, 4, 2	Ground						7 833.96		304
		6, 4, 2← 6, 4, 3	Ground						20 396.03		304
		7, 5, 2← 7, 5, 3	Ground						16 065.29		304
		8, 5, 3← 8, 5, 4	Ground						32 137.90		304
		8, 6, 2← 8, 6, 3	Ground						11 680.10		304
		9, 6, 3← 9, 6, 2	Ground						26 938.68		304
		10, 7, 3←10, 7, 4	Ground						21 229.43		304
		11, 8, 3←11, 8, 4	Ground						15 553.69		304
		12, 9, 3←12, 9, 4	Ground						10 487.08		304
$HN^{15}O_3^{16}$	33	1, 0, 1← 0, 0, 0	Ground						18 357.05		304
		1, 1, 1← 0, 0, 0	Ground						19 272.44		304
		2, 1, 2← 1, 0, 1	Ground						31 792.60		304
		2, 1, 2← 1, 1, 1	Ground						30 877.22		304

H_2O_2 $C_2(C_s,C_s)$ HOOH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$H_2O_2^{16}$	C_2	41	301 700. N	26 192. N	25 126. N				
$D_2O_2^{16}$	C_2	42	162 700. N	23 749. N	22 165. N				
HDO_2^{16}	C_1	43	210 800. N	25 047. N	23 501. N				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_1	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
41	0. X	0. X	2.26 M		113						

References:

ABC: 355 D_J: D_{JK}: κ: Δ:

μ: 93 eQq: V: 93 I: ω:

Add. Ref.: 57

Torsional frequency = 314 cm^{-1}. Ref: 315.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$H_2O_2^{16}$	41	Not Reported							11 072.4	.5	115
		Not Reported							14 829.5	.2	115
		Not Reported							16 032.	2.	115
		Not Reported							22 054.5	.2	115
		Not Reported							27 639.6	.2	115
		Not Reported							35 916.	2.	115
		Not Reported							37 517.6	.2	115
		Not Reported							39 033.	2.	115
		Not Reported							39 495.	2.	115
		Not Reported							39 760.	2.	115
$D_2O_2^{16}$	42	Not Reported							10 068.	3.	302
		Not Reported							10 209.	3.	302
		Not Reported							10 560.	3.	302
		Not Reported							11 112.	3.	302
		Not Reported							11 391.	3.	302
		Not Reported							11 460.	3.	302
		Not Reported							12 335.	3.	302
		Not Reported							13 366.	3.	302
		Not Reported							13 387.	3.	302
		Not Reported							13 628.	3.	302
		Not Reported							13 824.	3.	302
		Not Reported							14 340.	3.	302
		Not Reported							14 428.	3.	302
		Not Reported							14 453.	3.	302
		Not Reported							14 861.	3.	302
		Not Reported							15 068.	3.	302
		Not Reported							15 253.	3.	302
		Not Reported							15 570.	3.	302
		Not Reported							15 684.	3.	302
		Not Reported							15 890.	3.	302
		Not Reported							16 344.	3.	302
		Not Reported							16 483.	3.	302
		Not Reported							16 613.	3.	302
		Not Reported							16 803.	3.	302
		Not Reported							17 152.	3.	302
		Not Reported							19 322.	3.	302
		Not Reported							19 854.	3.	302
		Not Reported							20 728.	3.	302
		Not Reported							20 990.	3.	302
		Not Reported							22 725.	3.	302
		Not Reported							23 207.	3.	302
		Not Reported							23 571.	3.	302
		Not Reported							23 694.	3.	302
		Not Reported							24 152.	3.	302
		Not Reported							24 204.	3.	302
		Not Reported							24 545.	3.	302
		Not Reported							24 778.	3.	302
		Not Reported							25 040.	3.	302
		Not Reported							25 235.	3.	302
		Not Reported							25 560.	3.	302

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$D_2O_2^{16}$	42	Not Reported							25 680.	3.	302
		Not Reported							26 016.	3.	302
		Not Reported							26 549.	3.	302
		Not Reported							26 821.	3.	302
		Not Reported							27 005.	3.	302
		Not Reported							27 141.	3.	302
		Not Reported							27 152.	3.	302
		Not Reported							27 282.	3.	302
		Not Reported							27 645.	3.	302
		Not Reported							27 681.	3.	302
		Not Reported							27 830.	3.	302
		Not Reported							27 863.	3.	302
		Not Reported							27 899.	3.	302
		Not Reported							28 105.	3.	302
		Not Reported							28 373.	3.	302
		Not Reported							28 694.	3.	302
		Not Reported							28 793.	3.	302
		Not Reported							28 802.	3.	302
		Not Reported							29 017.	3.	302
		Not Reported							29 136.	3.	302
		Not Reported							29 453.	3.	302
		Not Reported							29 759.	3.	302
		Not Reported							29 962.	3.	302
		Not Reported							29 984.	3.	302
		Not Reported							30 134.	3.	302
		Not Reported							30 511.	3.	302
		Not Reported							30 739.	3.	302
		Not Reported							30 791.	3.	302
		Not Reported							30 878.	3.	302
		Not Reported							31 162.	3.	302
		Not Reported							31 181.	3.	302
		Not Reported							31 940.	3.	302
		Not Reported							32 234.	3.	302
		Not Reported							32 280.	3.	302
		Not Reported							32 708.	3.	302
		Not Reported							32 975.	3.	302
		Not Reported							34 348.	3.	302
		Not Reported							34 540.	3.	302
		Not Reported							34 583.	3.	302
		Not Reported							34 709.	3.	302
		Not Reported							34 785.	3.	302
		Not Reported							35 028.	3.	302
		Not Reported							35 466.	3.	302
		Not Reported							35 515.	3.	302
		Not Reported							35 560.	3.	302
		Not Reported							35 732.	3.	302
		Not Reported							35 975.	3.	302
		Not Reported							36 032.	3.	302
		Not Reported							36 105.	3.	302
		Not Reported							36 162.	3.	302

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$D_2O_2^{16}$	42	Not Reported							36 268.	3.	302
		Not Reported							36 482.	3.	302
		Not Reported							37 076.	3.	302
		Not Reported							37 582.	3.	302
		Not Reported							38 132.	3.	302
		Not Reported							38 304.	3.	302
		Not Reported							38 752.	3.	302
		Not Reported							38 799.	3.	302
		Not Reported							39 659.	3.	302
HDO_2^{16}	43	1, , ← 1, ,							14 503.	3.	302
		2, , ← 2, ,							13 032.	3.	302
		3, , ← 3, ,							10 836.	3.	302
		5, , ← 5, ,							37 526.	3.	302
		6, , ← 6, ,							37 096.	3.	302
		7, , ← 7, ,							36 575.	3.	302
		8, , ← 8, ,							10 336.	3.	302
		8, , ← 8, ,							35 992.	3.	302
		9, , ← 9, ,							16 382.	3.	302
		9, , ← 9, ,							35 332.	3.	302
		10, , ←10, ,							22 928.	3.	302
		10, , ←10, ,							34 598.	3.	302
		11, , ←11, ,							29 923.	3.	302
		11, , ←11, ,							33 790.	3.	302
		11, , ←11, ,							33 791.	3.	302
		12, , ←12, ,							32 915.	3.	302
		12, , ←12, ,							32 917.	3.	302
		12, , ←12, ,							37 313.	3.	302
		13, , ←13, ,							31 952.	3.	302
		13, , ←13, ,							31 956.	3.	302
		14, , ←14, ,							30 921.	3.	302
		14, , ←14, ,							30 928.	3.	302
		15, , ←15, ,							29 818.	3.	302
		15, , ←15, ,							29 830.	3.	302
		16, , ←16, ,							28 631.	3.	302
		16, , ←16, ,							28 651.	3.	302
		17, , ←17, ,							27 375.	3.	302
		17, , ←17, ,							27 406.	3.	302
		18, , ←18, ,							26 036.	3.	302
		18, , ←18, ,							26 084.	3.	302
		19, , ←19, ,							24 624.	3.	302
		19, , ←19, ,							24 707.	3.	302
		20, , ←20, ,							23 130.	3.	302
		20, , ←20, ,							23 252.	3.	302
		21, , ←21, ,							21 553.	3.	302
		21, , ←21, ,							21 730.	3.	302

H_4N_2 $C_2(C_s,C_s)$ H_2NNH_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$H_2N^{14}N^{14}H_2$	C_2	51			59 660. M	.0278	.059		

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_1	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
51	0. X	1.75 M	0. X	−4.09	1100	50					

References:

ABC: 346 D_J: 346 D_{JK}: 346 κ: Δ:

μ: 346 eQq: 346 V: 346 I: ω:

Add. Ref.: 241

Inversion barrier height = 2800 ± 150, cal/mol. Calculated rotational constants: $A_e + B_e = 48156.5 \pm .5$ MHz, $C_e = 119360 \pm 50$ MHz. Ref: 346.

Hydrazine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.[1]	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$H_2N^{14}N^{14}H_2$	51	1, 1← 2, 0	Ground	E	0		2		3	15 058.60	.05	346
		1, 1← 2, 0	Ground	E	0		1		2	15 059.51	.05	346
		1, 1← 2, 0	Ground	E	0		2		3	15 060.23	.05	346
		1, 1← 2, 0	Ground	E	0		3		4	15 061.12	.05	346
		1, 1← 2, 0	Ground	E	0		1		2	15 061.94	.05	346
		1, 1← 2, 0	Ground	E	0		1		1	15 062.65	.05	346
		1, 1← 2, 0	Ground	E	0		1		0	15 063.45	.05	346
		1, 1← 2, 0	Ground	E	0		2		3	15 064.36	.05	346
		1, 1← 2, 0	Ground	E	0		1		2	15 065.06	.05	346
		1, 1← 2, 0	Ground	E	0		2		3	15 066.02	.05	346
		1, 1← 2, 0	Ground	E	0		3		4	15 066.95	.05	346
		1, 1← 2, 0	Ground	E	0		1		2	15 067.55	.05	346
		1, 1← 2, 0	Ground	E	0		1		1	15 068.17	.05	346
		1, 1← 2, 0	Ground	E	0		1		0	15 069.35	.05	346
		1, 1← 2, 0	Ground	A	0					15 091.2		346
		1, 1← 2, 0	Ground	A	0					15 102.4		346
		1, 1← 2, 0	Ground							15 109.6	.05	346
		1, 1← 2, 0	Ground	A	0					31 064.3		346
		1, 1← 2, 0	Ground							31 070.3	.05	346
		1, 1← 2, 0	Ground	E	0		1		2	31 071.44	.05	346
		1, 1← 2, 0	Ground	E	0		2		3	31 072.25	.05	346
		1, 1← 2, 0	Ground	E	0		3		4	31 073.21	.05	346
		1, 1← 2, 0	Ground	E	0		1		2	31 073.95	.05	346
		1, 1← 2, 0	Ground	E	0		1		1	31 074.45	.05	346
		1, 1← 2, 0	Ground	A	0					31 075.5		346

[1] Rotational quantum numbers have been entered as given in reference, although hydrazine is not a symmetric top.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$H_2N^{14}N^{14}H_2$	51	1, 1← 2, 0	Ground	E	0		1		2	31 077.12	.05	346
		1, 1← 2, 0	Ground	E	0		2		3	31 077.85	.05	346
		1, 1← 2, 0	Ground	E	0		3		4	31 078.95	.05	346
		1, 1← 2, 0	Ground	E	0		1		2	31 079.52	.05	346
		1, 1← 2, 0	Ground	E	0		1		1	31 080.20	.05	346
		3, 0← 2, 1	Ground	E	0		4		4	17 072.48	.05	346
		3, 0← 2, 1	Ground	E	0		4		3	17 073.08	.05	346
		3, 0← 2, 1	Ground	E	0		5		4	17 073.60	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	17 074.14	.05	346
		3, 0← 2, 1	Ground	E	0		1		1	17 074.48	.05	346
		3, 0← 2, 1	Ground	E	0		3		3	17 075.10	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	17 075.84	.05	346
		3, 0← 2, 1	Ground	E	0		4		4	17 078.11	.05	346
		3, 0← 2, 1	Ground	E	0		4		3	17 078.78	.05	346
		3, 0← 2, 1	Ground	E	0		5		4	17 079.35	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	17 079.81	.05	346
		3, 0← 2, 1	Ground	E	0		1		1	17 080.10	.05	346
		3, 0← 2, 1	Ground	E	0		3		3	17 080.85	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	17 081.33	.05	346
		3, 0← 2, 1	Ground							17 086.3	.05	346
		3, 0← 2, 1	Ground	A	0					17 092.7		346
		3, 0← 2, 1	Ground	A	0					17 104.1		346
		3, 0← 2, 1	Ground							33 033.0	.05	346
		3, 0← 2, 1	Ground	A	0					33 054.2		346
		3, 0← 2, 1	Ground	A	0					33 065.4		346
		3, 0← 2, 1	Ground	E	0		4		4	33 077.98	.05	346
		3, 0← 2, 1	Ground	E	0		4		3	33 078.78	.05	346
		3, 0← 2, 1	Ground	E	0		5		4	33 079.36	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	33 079.80	.05	346
		3, 0← 2, 1	Ground	E	0		1		1	33 080.14	.05	346
		3, 0← 2, 1	Ground	E	0		3		3	33 080.78	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	33 081.36	.05	346
		3, 0← 2, 1	Ground	E	0		4		4	33 083.82	.05	346
		3, 0← 2, 1	Ground	E	0		4		3	33 084.28	.05	346
		3, 0← 2, 1	Ground	E	0		5		4	33 084.90	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	33 085.52	.05	346
		3, 0← 2, 1	Ground	E	0		1		1	33 085.78	.05	346
		3, 0← 2, 1	Ground	E	0		3		3	33 086.44	.05	346
		3, 0← 2, 1	Ground	E	0		3		2	33 087.04	.05	346
		6, 2← 7, 1	Ground	A	0					12 946.7		346
		6, 2← 7, 1	Ground	A	0					12 958.1		346
		6, 2← 7, 1	Ground							13 113.3	.05	346
		6, 2← 7, 1	Ground	A	0					13 279.8		346
		6, 2← 7, 1	Ground	A	0					13 291.3		346
		6, 2← 7, 1	Ground	A	0					28 844.2		346
		6, 2← 7, 1	Ground	A	0					28 855.4		346
		6, 2← 7, 1	Ground							29 053.6	.05	346
		6, 2← 7, 1	Ground	A	0					29 240.3		346
		6, 2← 7, 1	Ground	A	0					29 251.8		346
		8, 1← 7, 2	Ground	A	0					18 831.1		346

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$H_2N^{14}N^{14}H_2$	51	8, 1← 7, 2	Ground	A	0					18 842.2		346
		8, 1← 7, 2	Ground							19 086.1	.05	346
		8, 1← 7, 2	Ground	A	0					19 341.1		346
		8, 1← 7, 2	Ground	A	0					19 352.5		346
		8, 1← 7, 2	Ground	A	0					34 778.6		346
		8, 1← 7, 2	Ground	A	0					34 790.4		346
		8, 1← 7, 2	Ground							35 004.7	.05	346
		8, 1← 7, 2	Ground	A	0					35 207.8		346
		8, 1← 7, 2	Ground	A	0					35 219.0		346
		9, 1← 8, 2	Ground	A	0					66 902.0	.05	346
		9, 1← 8, 2	Ground	A	0					67 540.1	.05	346
		11, 3←12, 2	Ground	A	0					11 351.4		346
		11, 3←12, 2	Ground	A	0					11 363.0		346
		11, 3←12, 2	Ground	A	0					26 883.9		346
		11, 3←12, 2	Ground	A	0					26 895.4		346
		11, 3←12, 2	Ground	A	0					26 934.0		346
		11, 3←12, 2	Ground	A	0					26 945.4		346
		13, 2←12, 3	Ground	A	0					21 153.6		346
		13, 2←12, 3	Ground	A	0					21 165.4		346
		13, 2←12, 3	Ground	A	0					21 221.7		346
		13, 2←12, 3	Ground	A	0					21 233.4		346
		13, 2←12, 3	Ground	A	0					36 647.1		346
		13, 2←12, 3	Ground	A	0					36 658.7		346
		13, 2←12, 3	Ground	A	0					36 717.4		346
		13, 2←12, 3	Ground	A	0					36 729.0		346
		Not Reported								4 764.0		218
		Not Reported								4 879.4		218
		Not Reported								5 386.0		218
		Not Reported								5 562.53		218
		Not Reported								5 568.98		218
		Not Reported								5 992.		218
		Not Reported								6 144.		218
		Not Reported								6 498.3		218
		Not Reported								6 575.71		218
		Not Reported								6 588.6		218
		Not Reported								6 759.91		218
		Not Reported								7 444.9		218
		Not Reported								7 977.76		218
		Not Reported								8 134.63		218
		Not Reported								8 147.09		218
		Not Reported								8 270.73		218
		Not Reported								8 273.57		218
		Not Reported								8 478.7		218
		Not Reported								8 824.0		218
		Not Reported								9 227.5		218
		Not Reported								9 543.51		218
		Not Reported								9 555.23		218
		Not Reported								9 689.62		218
		Not Reported								9 689.72		218
		Not Reported								9 689.80		218

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$H_2N^{14}N^{14}H_2$	51	Not Reported							9 697.59		218
		Not Reported							11 351.2		218
		Not Reported							11 351.56		218
		Not Reported							11 388.0		218
		Not Reported							11 390.0		218
		Not Reported							11 406.2		218
		Not Reported							11 413.67		218
		Not Reported							12 424.12		218
		Not Reported							12 772.8		218
		Not Reported							13 151.3		218
		Not Reported							13 191.71		218
		Not Reported							13 192.5		218
		Not Reported							13 193.29		218
		Not Reported							13 194.13		218
		Not Reported							13 279.22		218
		Not Reported							13 280.02		218
		Not Reported							13 422.6		218
		Not Reported							13 542.53		218
		Not Reported							13 557.30		218
		Not Reported							13 632.40		218
		Not Reported							13 988.41		218
		Not Reported							14 065.4		218
		Not Reported							14 441.59		218
		Not Reported							14 475.4		218
		Not Reported							14 556.31		218
		Not Reported							14 570.8		218
		Not Reported							14 687.29		218
		Not Reported							14 700.4		218
		Not Reported							14 900.5		218
		Not Reported							15 099.30		218
		Not Reported							15 099.86		218
		Not Reported							15 100.72		218
		Not Reported							15 101.32		218
		Not Reported							15 103.40		218
		Not Reported							15 104.37		218
		Not Reported							15 892.15		218
		Not Reported							15 921.66		218
		Not Reported							16 045.67		218
		Not Reported							16 286.4		218
		Not Reported							16 313.92		218
		Not Reported							16 376.94		218
		Not Reported							16 698.20		218
		Not Reported							16 767.90		218
		Not Reported							17 071.6		218
		Not Reported							17 077.2		218
		Not Reported							17 092.35		218
		Not Reported							17 103.84		218
		Not Reported							17 105.42		218
		Not Reported							17 125.84		218
		Not Reported							17 326.69		218

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$H_2N^{14}N^{14}H_2$	51	Not Reported							17 332.72		218
		Not Reported							17 797.71		218
		Not Reported							17 865.95		218
		Not Reported							18 086.02		218
		Not Reported							18 118.9		218
		Not Reported							18 663.70		218
		Not Reported							18 687.31		218
		Not Reported							18 691.44		218
		Not Reported							18 781.43		218
		Not Reported							18 824.0		218
		Not Reported							18 830.96		218
		Not Reported							18 940.14		218
		Not Reported							19 088.39		218
		Not Reported							19 118.8		218
		Not Reported							19 125.6		218
		Not Reported							19 126.2		218
		Not Reported							19 126.93		218
		Not Reported							19 127.65		218
		Not Reported							19 128.86		218
		Not Reported							19 129.54		218
		Not Reported							19 129.88		218
		Not Reported							19 352.65		218
		Not Reported							19 353.0		218
		Not Reported							19 488.29		218
		Not Reported							19 502.92		218
		Not Reported							19 559.0		218
		Not Reported							19 561.4		218
		Not Reported							19 672.93		218
		Not Reported							19 804.8		218
		Not Reported							19 806.06		218
		Not Reported							19 874.46		218
		Not Reported							19 875.04		218
		Not Reported							19 945.6		218
		Not Reported							20 073.28		218
		Not Reported							20 073.78		218
		Not Reported							20 414.9		218
		Not Reported							20 797.01		218
		Not Reported							20 950.65		218
		Not Reported							21 107.10		218
		Not Reported							21 110.25		218
		Not Reported							21 127.0		218
		Not Reported							21 236.46		218
		Not Reported							21 239.52		218
		Not Reported							21 527.14		218
		Not Reported							21 661.71		218
		Not Reported							22 235.35		218
		Not Reported							22 413.3		218
		Not Reported							22 516.50		218
		Not Reported							22 766.98		218
		Not Reported							22 779.30		218

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$H_2N^{14}N^{14}H_2$	51	Not Reported							22 839.43		218
		Not Reported							22 839.91		218
		Not Reported							22 902.87		218
		Not Reported							23 119.2		218
		Not Reported							23 130.70		218
		Not Reported							23 131.19		218
		Not Reported							23 230.27		218
		Not Reported							23 771.02		218
		Not Reported							24 120.0		218
		Not Reported							24 285.79		218
		Not Reported							24 286.23		218
		Not Reported							24 377.18		218
		Not Reported							24 824.59		218
		Not Reported							24 923.34		218
		Not Reported							24 935.41		218
		Not Reported							25 078.38		218
		Not Reported							25 201.35		218
		Not Reported							25 213.53		218
		Not Reported							26 162.06		218
		Not Reported							26 346.36		218
		Not Reported							26 605.60		218
		Not Reported							26 872.2		218
		Not Reported							26 874.2		218
		Not Reported							26 937.28		218
		Not Reported							26 950.5		218
		Not Reported							26 992.83		218
		Not Reported							26 995.23		218
		Not Reported							27 027.4		218
		Not Reported							27 088.7		218
		Not Reported	Ground						28 002.87		218
		Not Reported	Ground						28 025.6		218
		Not Reported	Ground						28 207.9		218
		Not Reported	Ground						28 218.66		218
		Not Reported	Ground						28 222.08		218
		Not Reported	Ground						28 830.5		218
		Not Reported	Ground						28 855.75		218
		Not Reported	Ground						28 933.1		218
		Not Reported	Ground						29 010.24		218
		Not Reported	Ground						29 011.74		218
		Not Reported	Ground						29 012.73		218
		Not Reported	Ground						29 199.6		218
		Not Reported	Ground						29 251.64		218
		Not Reported	Ground						29 252.01		218
		Not Reported	Ground						29 491.6		218

CF_3S $C_s(C_{3v},C_{4v})$ CF_3SF_5

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}F_3^{19}S^{32}F_5^{19}$	C_s	61	1 097.6 M	1 097.6 M					

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
61					220						

References:

ABC: 55 D_J: D_{JK}: κ: Δ:

μ: eQq: V: 55 I: ω:

Torsional frequency = 93.5 ± 25 cm^{-1}. V_{12} = 219 ± 120 cm^{-1}. Ref: 55.

No Spectral Lines

CH_2O_2 $C_s(C_s,C_s)$ HCOOH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$HC^{12}O^{16}O^{16}H$	C_s	71	77 520.07 M	12 054.98 M	10 416.16 M	.00928	−.0830		.126
$HC^{12}O^{16}O^{16}D$	C_s	72	66 110. M	11 762.55 M	9 970.05 M	.01042	−.0575		
$DC^{12}O^{16}O^{16}H$	C_s	73	57 710. M	12 055.80 M	9 955.71 M	.00845	−.0366		
$DC^{12}O^{16}O^{16}D$	C_s	74	50 815. M	11 759.80 M	9 534.15 M	.00837	−.0309		
$HC^{13}O^{16}O^{16}H$	C_s	75		12 053.7 M	10 378.9 M				
$HC^{12}O^{18}O^{16}H$	C_s	76	76 521. M	11 396.91 M	9 904.76 M				
$HC^{12}O^{16}O^{18}H$	C_s	77	77 206. M	11 383.58 M	9 906.06 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_1	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
71	1.391 M	0.26 M	0. X		17000						
72	1.377 M	0.22 M	0. X								
75	1.415 T										

References:

ABC: 179, 199, 235, 291, 305 D_J: 305 D_{JK}: 305 κ: Δ: 235

μ: 235, 347 eQq: V: 179 I: ω:

Add. Refs.: 31, 46, 87, 110, 131, 156, 157

For species 71, the centrifugal distortion is : $D_K = 3.12$ MHz. Ref: 305. Its torsional frequency $= 667 \pm 41$ cm^{-1}. Ref: 179. The centrifugal distortion for species 72 is: $D_K = 1.77$ MHz; for species 73 is: $D_K = 1.21$ MHz; and for species 74 is $D_K = .75$ MHz. Ref: 305.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$HC^{12}O^{16}O^{16}H$	71	1, 0, 1← 0, 0, 0							22 471.22	.1	210
		1, 1, 1← 2, 0, 2							20 543.96		235
		2, 0, 2← 1, 0, 1							44 911.68	.28	199
		2, 1, 1← 1, 1, 0							46 581.22	.29	199
		2, 1, 2← 1, 1, 1							43 303.62	.27	199
		3, 0, 3← 2, 0, 2							67 291.05	.41	199
		3, 1, 2← 2, 1, 1							69 852.03	.42	199
		3, 1, 3← 2, 1, 2							64 936.26	.40	199
		3, 2, 1← 2, 2, 0							67 536.09	.41	199
		3, 2, 2← 2, 2, 1							67 414.80	.41	199
		3, 1, 2← 3, 1, 3							9 831.98		235
		4, 0, 4← 3, 0, 3							89 579.18	.53	199
		4, 0, 4← 3, 1, 3							28 086.39		235
		4, 1, 3← 3, 1, 2							93 098.46	.56	199
		4, 1, 4← 3, 1, 3							86 545.92	.52	199
		4, 2, 2← 3, 2, 1							90 164.52	.54	199
		4, 2, 3← 3, 2, 2							89 861.52	.54	199
		4, 3, 1← 3, 3, 0							89 950.34	.54	199
		4, 3, 2← 3, 3, 1							89 948.32	.54	199
		4, 1, 3← 4, 1, 4							16 382.2		200
		5, 0, 5← 4, 0, 4							111 746.65	.68	199
		5, 1, 4← 4, 1, 3							116 311.35	.70	199
		5, 1, 5← 4, 1, 4							108 127.00	.65	199
		5, 2, 3← 4, 2, 2							112 891.75	.68	199
		5, 2, 4← 4, 2, 3							112 287.29	.68	199
		5, 3, 2← 4, 3, 1							112 467.04	.68	199
		5, 3, 3← 4, 3, 2							112 459.70	.68	199
		5, 4, 1← 4, 4, 0							112 432.60	.68	199
		5, 4, 2← 4, 4, 1							112 432.60	.68	199
		5, 1, 4← 5, 1, 5							24 568.99	.03	200
		6, 0, 6← 5, 0, 5							133 767.06	.81	199
		6, 1, 5← 5, 1, 4							139 481.70	.84	199
		6, 1, 6← 5, 1, 5							129 671.70	.78	199
		6, 2, 4← 5, 2, 3							135 737.70	.82	199
		6, 2, 5← 5, 2, 4							134 686.20	.82	199
		6, 3, 3← 5, 3, 2							135 004.74	.82	199
		6, 3, 4← 5, 3, 3							134 985.36	.82	199
		6, 4, 2← 5, 4, 1							134 938.26	.82	199
		6, 4, 3← 5, 4, 2							134 938.26	.82	199
		6, 5, 1← 5, 5, 0							134 920.32	.82	199
		6, 5, 2← 5, 5, 1							134 920.32	.82	199
		6, 1, 5← 6, 1, 6							34 378.86		235
		7, 0, 7← 6, 0, 6							155 617.9	.1	210
		7, 1, 6← 6, 1, 5							162 598.4	.1	210
		7, 1, 7← 6, 1, 6							151 176.1	.1	210
		7, 2, 5← 6, 2, 4							158 721.0	.1	210
		7, 2, 6← 6, 2, 5							157 054.0	.1	210
		7, 3, 4← 6, 3, 3							157 570.6	.1	210
		7, 3, 5← 6, 3, 4							157 526.1	.1	210
		7, 4, 3← 6, 4, 2							157 455.2	.1	210

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$HC^{12}O^{16}O^{16}H$	71	7, 4, 4← 6, 4, 3							157 455.2	.1	210
		7, 5, ← 6, 5,							157 422.7	.1	210
		7, 6, ← 6, 6,							157 412.9	.1	210
		7, 1, 6← 7, 1, 7							45 801.13		235
		8, 0, 8← 7, 0, 7							177 283.0	.1	210
		8, 1, 7← 7, 1, 6							185 650.3	.1	210
		8, 1, 8← 7, 1, 7							172 636.7	.1	210
		8, 2, 6← 7, 2, 5							181 850.2	.1	210
		8, 2, 7← 7, 2, 6							179 384.6	.1	210
		8, 3, 5← 7, 3, 4							180 171.4	.1	210
		8, 3, 6← 7, 3, 5							180 083.0	.1	210
		8, 4, 4← 7, 4, 3							179 985.3	.1	210
		8, 4, 5← 7, 4, 4							179 984.1	.1	210
		8, 5, ← 7, 5,							179 932.2	.1	210
		8, 1, 7← 8, 1, 8							58 815.46		235
		9, 0, 9← 8, 0, 8							198 755.7	.1	210
		9, 2, 7← 8, 2, 6							205 127.9	.1	210
		9, 2, 8← 8, 2, 7							201 673.6	.1	210
		9, 3, 6← 8, 3, 5							202 815.4	.1	210
		9, 3, 7← 8, 3, 6							202 654.0	.1	210
		9, 4, 5← 8, 4, 4							202 530.0	.1	210
		9, 4, 6← 8, 4, 5							202 527.3	.1	210
		9, 5, 4← 8, 5, 3							202 449.9	.1	210
		9, 5, 5← 8, 5, 4							202 449.9	.1	210
		9, 6, ← 8, 6,							202 418.2	.1	210
		9, 7, ← 8, 7,							202 409.6	.1	210
		9, 8, ← 8, 8,							202 413.8	.1	210
		9, 2, 7← 9, 2, 8							9 696.83		235
		11, 2, 9←11, 2,10							20 297.88		235
		12, 2,10←12, 2,11							27 758.05		235
		13, 2,11←13, 2,12							36 830.		235
		16, 3,13←16, 3,14							8 968.50		235
		18, 3,15←18, 3,16							17 286.		235
		19, 3,16←19, 3,17							23 203.41		235
		20, 3,17←20, 3,18							30 523.12		235
		24, 4,20←24, 4,21							9 410.		235
		27, 4,23←27, 4,24							22 326.42		235
		28, 4,24←28, 4,25							28 935.		235
		29, 4,25←29, 4,26							36 915.		235
		32, 5,27←32, 5,28							8 662.		235
		33, 5,28←33, 5,29							11 512.		235
		Not Reported							16 989.	5.	67
		Not Reported							24 595.	5.	67
		Not Reported							25 218.	5.	67
		Not Reported							26 342.	5.	67
$HC^{12}O^{16}O^{16}D$	72	1, 0, 1← 0, 0, 0	Ground						21 732.72	.10	100
		2, 0, 2← 1, 0, 1	Ground						43 421.36	.20	100
		2, 1, 1← 1, 1, 0	Ground						45 257.40	.20	100
		2, 1, 2← 1, 1, 1	Ground						41 672.98	.20	100
		5, 1, 5← 5, 1, 4	Ground						26 865.5	.3	179

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$HC^{12}O^{16}O^{16}D$	72	7, 0, 7← 6, 0, 6	Ground						149 753.66	.2	305
		7, 1, 6← 6, 1, 5	Ground						157 770.81	.2	305
		7, 1, 7← 6, 1, 6	Ground						145 312.14	.2	305
		7, 2, 5← 6, 2, 4	Ground						154 137.58	.2	305
		7, 2, 6← 6, 2, 5	Ground						151 778.74	.2	305
		7, 3, 4← 6, 3, 3	Ground						152 526.01	.2	305
		7, 3, 5← 6, 3, 4	Ground						152 442.80	.2	305
		7, 4, 3← 6, 4, 2	Ground						152 344.38	.2	305
		7, 4, 4← 6, 4, 3	Ground						152 343.36	.2	305
		7, 5, ← 6, 5,	Ground						152 288.87	.2	305
		7, 6, ← 6, 6,	Ground						152 264.95	.2	305
$DC^{12}O^{16}O^{16}H$	73	1, 0, 1← 0, 0, 0	Ground						22 011.3	.3	179
		2, 1, 1← 1, 1, 0	Ground						46 122.6	.6	179
		2, 1, 2← 1, 1, 1	Ground						41 923.0	.6	179
		4, 1, 4← 4, 1, 3	Ground						20 989.6	.3	179
		7, 0, 7← 6, 0, 6	Ground						150 345.06	.2	305
		7, 1, 6← 6, 1, 5	Ground						160 392.07	.2	305
		7, 1, 7← 6, 1, 6	Ground						145 882.95	.2	305
		7, 2, 5← 6, 2, 4	Ground						157 241.48	.2	305
		7, 2, 6← 6, 2, 5	Ground						153 521.68	.2	305
		7, 3, 4← 6, 3, 3	Ground						154 757.18	.2	305
		7, 3, 5← 6, 3, 4	Ground						154 571.17	.2	305
		7, 4, 2← 6, 4, 2	Ground						154 431.13	.2	305
		7, 4, 4← 6, 4, 3	Ground						154 427.84	.2	305
		7, 5, ← 6, 5,	Ground						154 332.94	.2	305
		7, 6, ← 6, 6,	Ground						154 285.66	.2	305
$DC^{12}O^{16}O^{16}D$	74	1, 0, 1← 0, 0, 0	Ground						21 293.9	.3	179
		2, 1, 1← 1, 1, 0	Ground						44 813.4	.6	179
		4, 1, 4← 4, 1, 3	Ground						22 237.5	.3	179
		6, 0, 6← 5, 0, 5	Ground						124 685.34	.2	305
		6, 1, 5← 5, 1, 4	Ground						133 623.69	.2	305
		6, 1, 6← 5, 1, 5	Ground						120 407.60	.2	305 [1]
		6, 2, 4← 5, 2, 3	Ground						130 411.85	.2	305
		6, 2, 5← 5, 2, 4	Ground						127 342.80	.2	305
		6, 3, 3← 5, 3, 2	Ground						128 336.34	.2	305
		6, 3, 4← 5, 3, 3	Ground						128 203.04	.2	305
		6, 4, 2← 5, 4, 1	Ground						128 077.64	.2	305
		6, 4, 3← 5, 4, 2	Ground						128 075.90	.2	305
		6, 5, ← 5, 5,	Ground						127 996.80	.2	305
$HC^{13}O^{16}O^{16}H$	75	1, 0, 1← 0, 0, 0	Ground						22 432.6	.3	179
		2, 1, 2← 1, 1, 1	Ground						43 190.4	.6	179
$HC^{12}O^{18}O^{16}H$	76	1, 0, 1← 0, 0, 0	Ground						21 301.67	.1	291
		2, 1, 1← 1, 1, 0	Ground						44 095.5	.2	291
		4, 1, 4← 4, 1, 3	Ground						14 919.20	.1	291
		5, 1, 5← 5, 1, 4	Ground						22 372.49	.1	291
		6, 1, 6← 6, 1, 5	Ground						31 309.00	.1	291
$HC^{12}O^{16}O^{18}H$	77	1, 0, 1← 0, 0, 0	Ground						21 289.64	.1	291
		2, 1, 1← 1, 1, 0	Ground						44 056.8	.2	291
		4, 1, 4← 4, 1, 3	Ground						14 773.56	.1	291
		5, 1, 5← 5, 1, 4	Ground						22 154.85	.1	291
		6, 1, 6← 6, 1, 5	Ground						31 003.73	.1	291

[1] Mirri's report of a $6_{66} \leftarrow 5_{15}$ transition for DCOOD obviously involves a typographical error: the transition has been entered as $6_{16} \leftarrow 5_{15}$.

CH_3AsF_2 $C_s(C_{3v},C_s)$ CH_3AsF_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3As^{75}F_2^{19}$	C_s	81	5 414.49 M	5 318.28 M	3 871.88 M	−3.7	−5.45		

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
81	2.88[1] L	0. X		−220	1330						

1. The value given was determined from benzene solutions of the compound, quoted from McClellan's Tables of Experimental Dipole Moments.

References:

ABC: 329 D_J: 329 D_{JK}: 329 κ: Δ:

μ: 364 eQq: 329 V: 344 I: ω:

Centrifugal distortion (A-states): $D_K = 2.82 \pm .32 \times 10^{-3}$ MHz. Coupling parameter: $I_\alpha = 3.210 \pm .040$ amu Å^2. Ref: 329.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	3, 0, 3← 2, 0, 2	Ground	A	0		5/2		5/2	24 733.01	.2	329
		3, 0, 3← 2, 0, 2	Ground	E	0		9/2		7/2	24 748.55	.2	329
		3, 0, 3← 2, 0, 2	Ground	A	0		9/2		7/2	24 750.91	.2	329
		3, 0, 3← 2, 0, 2	Ground	E	0		9/2		7/2	24 752.13	.2	329
		3, 0, 3← 2, 0, 2	Ground	A	0		3/2		1/2	24 757.70	.2	329
		3, 0, 3← 2, 0, 2	Ground	E	0		7/2		5/2	24 761.98	.2	329
		3, 0, 3← 2, 0, 2	Ground	A	0		7/2		5/2	24 764.87	.2	329
		3, 0, 3← 2, 0, 2	Ground	E	0		7/2		5/2	24 766.40	.2	329
		3, 0, 3← 2, 0, 2	Ground	E	0		5/2		3/2	24 769.26	.2	329
		3, 0, 3← 2, 0, 2	Ground	A	0		5/2		3/2	24 771.88	.2	329
		3, 0, 3← 2, 0, 2	Ground	A	0		7/2		7/2	24 819.80	.2	329
		3, 1, 3← 2, 1, 2	Ground	A	0		5/2		5/2	24 733.01	.2	329
		3, 1, 3← 2, 1, 2	Ground	E	0		9/2		7/2	24 748.55	.2	329
		3, 1, 3← 2, 1, 2	Ground	A	0		9/2		7/2	24 750.91	.2	329
		3, 1, 3← 2, 1, 2	Ground	E	0		9/2		7/2	24 752.13	.2	329
		3, 1, 3← 2, 1, 2	Ground	A	0		3/2		1/2	24 757.70	.2	329
		3, 1, 3← 2, 1, 2	Ground	E	0		7/2		5/2	24 761.98	.2	329
		3, 1, 3← 2, 1, 2	Ground	A	0		7/2		5/2	24 764.87	.2	329
		3, 1, 3← 2, 1, 2	Ground	E	0		7/2		5/2	24 766.40	.2	329
		3, 1, 3← 2, 1, 2	Ground	E	0		5/2		3/2	24 769.26	.2	329
		3, 1, 3← 2, 1, 2	Ground	A	0		5/2		3/2	24 771.88	.2	329
		3, 1, 3← 2, 1, 2	Ground	A	0		7/2		7/2	24 819.80	.2	329
		4, 0, 4← 3, 0, 3	Ground	E	0		11/2		9/2	32 494.96	.2	329
		4, 0, 4← 3, 0, 3	Ground	A	0		11/2		9/2	32 497.75	.2	329
		4, 0, 4← 3, 0, 3	Ground	A	0		5/2		3/2	32 502.80	.2	329
		4, 0, 4← 3, 0, 3	Ground	A	0		9/2		7/2	32 506.10	.2	329
		4, 1, 4← 3, 1, 3	Ground	E	0		11/2		9/2	32 494.96	.2	329
		4, 1, 4← 3, 1, 3	Ground	A	0		11/2		9/2	32 497.75	.2	329
		4, 1, 4← 3, 1, 3	Ground	A	0		5/2		3/2	32 502.80	.2	329
		4, 1, 4← 3, 1, 3	Ground	A	0		9/2		7/2	32 506.10	.2	329
		7, 2, 5← 7, 2, 6	Ground	A	0		17/2		17/2	16 797.27	.05	329
		7, 2, 5← 7, 2, 6	Ground	A	0		11/2		11/2	16 803.68	.05	329
		7, 3, 5← 7, 1, 6	Ground	A	0		17/2		17/2	16 797.27	.05	329
		7, 3, 5← 7, 1, 6	Ground	A	0		11/2		11/2	16 803.68	.05	329
		7, 3, 4← 7, 3, 5	Ground	A	0		17/2		17/2	13 741.67	.05	329
		7, 3, 4← 7, 3, 5	Ground	A	0		11/2		11/2	13 747.12	.05	329
		7, 4, 4← 7, 2, 5	Ground	A	0		17/2		17/2	13 741.67	.05	329
		7, 4, 4← 7, 2, 5	Ground	A	0		11/2		11/2	13 747.12	.05	329
		8, 4, 4← 8, 4, 5	Ground	A	0		19/2		19/2	13 737.52	.05	329
		8, 4, 4← 8, 4, 5	Ground	A	0		13/2		13/2	13 741.32	.05	329
		8, 5, 4← 8, 3, 5	Ground	A	0		19/2		19/2	13 737.52	.05	329
		8, 5, 4← 8, 3, 5	Ground	A	0		13/2		13/2	13 741.32	.05	329
		9, 4, 5← 9, 4, 6	Ground	A	0		21/2		21/2	16 788.91	.05	329
		9, 4, 5← 9, 4, 6	Ground	A	0		15/2		15/2	16 792.16	.05	329
		9, 5, 5← 9, 3, 6	Ground	A	0		21/2		21/2	16 788.91	.05	329
		9, 5, 5← 9, 3, 6	Ground	A	0		15/2		15/2	16 792.16	.05	329
		10, 4, 6←10, 4, 7	Ground	E	0		17/2		17/2	19 839.13	.05	329
		10, 4, 6←10, 4, 7	Ground	A	0		23/2		23/2	19 839.97	.05	329
		10, 4, 6←10, 4, 7	Ground	A	0		17/2		17/2	19 842.75	.05	329
		10, 4, 6←10, 4, 7	Ground	E	0		17/2		17/2	19 843.71	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	10, 5, 6←10, 3, 7	Ground	E	0		17/2		17/2	19 839.13	.05	329
		10, 5, 6←10, 3, 7	Ground	A	0		23/2		23/2	19 839.97	.05	329
		10, 5, 6←10, 3, 7	Ground	A	0		17/2		17/2	19 842.75	.05	329
		10, 5, 6←10, 3, 7	Ground	E	0		17/2		17/2	19 843.71	.05	329
		10, 5, 5←10, 5, 6	Ground	A	0		23/2		23/2	16 785.12	.05	329
		10, 5, 5←10, 5, 6	Ground	A	0		17/2		17/2	16 787.50	.05	329
		10, 6, 5←10, 4, 6	Ground	A	0		23/2		23/2	16 785.12	.05	329
		10, 6, 5←10, 4, 6	Ground	A	0		17/2		17/2	16 787.50	.05	329
		10, 6, 4←10, 6, 5	Ground	A	0		23/2		23/2	13 728.97	.05	329
		10, 6, 4←10, 6, 5	Ground	A	0		17/2		17/2	13 730.97	.05	329
		10, 7, 4←10, 5, 5	Ground	A	0		23/2		23/2	13 728.97	.05	329
		10, 7, 4←10, 5, 5	Ground	A	0		17/2		17/2	13 730.97	.05	329
		11, 5, 6←11, 5, 7	Ground	E	0		19/2		19/2	19 834.67	.05	329
		11, 5, 6←11, 5, 7	Ground	A	0		25/2		25/2	19 836.16	.05	329
		11, 5, 6←11, 5, 7	Ground	A	0		19/2		19/2	19 838.21	.05	329
		11, 5, 6←11, 5, 7	Ground	E	0		19/2		19/2	19 839.13	.05	329
		11, 6, 6←11, 4, 7	Ground	E	0		19/2		19/2	19 834.67	.05	329
		11, 6, 6←11, 4, 7	Ground	A	0		25/2		25/2	19 836.16	.05	329
		11, 6, 6←11, 4, 7	Ground	A	0		19/2		19/2	19 838.21	.05	329
		11, 6, 6←11, 4, 7	Ground	E	0		19/2		19/2	19 839.13	.05	329
		11, 6, 5←11, 6, 6	Ground	A	0		25/2		25/2	16 781.11	.05	329
		11, 6, 5←11, 6, 6	Ground	A	0		19/2		19/2	16 782.95	.05	329
		11, 7, 5←11, 5, 6	Ground	A	0		25/2		25/2	16 781.11	.05	329
		11, 7, 5←11, 5, 6	Ground	A	0		19/2		19/2	16 782.95	.05	329
		11, 7, 4←11, 7, 5	Ground	A	0		25/2		25/2	13 723.91	.05	329
		11, 8, 4←11, 6, 5	Ground	A	0		25/2		25/2	13 723.91	.05	329
		12, 6, 6←12, 6, 7	Ground	A	0		27/2		27/2	19 832.22	.05	329
		12, 6, 6←12, 6, 7	Ground	A	0		21/2		21/2	19 833.84	.05	329
		12, 7, 6←12, 5, 7	Ground	A	0		27/2		27/2	19 832.22	.05	329
		12, 7, 6←12, 5, 7	Ground	A	0		21/2		21/2	19 833.84	.05	329
		12, 7, 5←12, 7, 6	Ground	E	0		27/2		27/2	16 773.67	.05	329
		12, 7, 5←12, 7, 6	Ground	E	0		21/2		21/2	16 775.09	.05	329
		12, 7, 5←12, 7, 6	Ground	A	0		27/2		27/2	16 776.75	.05	329
		12, 7, 5←12, 7, 6	Ground	E	0		27/2		27/2	16 777.84	.05	329
		12, 7, 5←12, 7, 6	Ground	A	0		21/2		21/2	16 778.19	.05	329
		12, 7, 5←12, 7, 6	Ground	E	0		21/2		21/2	16 779.21	.05	329
		12, 8, 5←12, 6, 6	Ground	E	0		27/2		27/2	16 773.67	.05	329
		12, 8, 5←12, 6, 6	Ground	E	0		21/2		21/2	16 775.09	.05	329
		12, 8, 5←12, 6, 6	Ground	A	0		27/2		27/2	16 776.75	.05	329
		12, 8, 5←12, 6, 6	Ground	E	0		27/2		27/2	16 777.84	.05	329
		12, 8, 5←12, 6, 6	Ground	A	0		21/2		21/2	16 778.19	.05	329
		12, 8, 5←12, 6, 6	Ground	E	0		21/2		21/2	16 779.21	.05	329
		13, 7, 6←13, 7, 7	Ground	A	0		29/2		29/2	19 827.98	.05	329
		13, 7, 6←13, 7, 7	Ground	A	0		23/2		23/2	19 829.30	.05	329
		13, 8, 6←13, 6, 7	Ground	A	0		29/2		29/2	19 827.98	.05	329
		13, 8, 6←13, 6, 7	Ground	A	0		23/2		23/2	19 829.30	.05	329
		13, 8, 5←13, 8, 6	Ground	A	0		23/2		23/2	16 773.02	.05	329
		13, 9, 5←13, 7, 6	Ground	A	0		23/2		23/2	16 773.02	.05	329
		14, 8, 6←14, 8, 7	Ground	A	0		31/2		31/2	19 823.39	.05	329
		14, 8, 6←14, 8, 7	Ground	A	0		25/2		25/2	19 824.47	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	14, 9, 6←14, 7, 7	Ground	A	0		31/2		31/2	19 823.39	.05	329
		14, 9, 6←14, 7, 7	Ground				25/2		25/2	19 824.47	.05	329
		15, 9, 6←15, 9, 7	Ground	A	0		31/2		31/2	19 809.09	.05	329
		15, 9, 6←15, 9, 7	Ground	A	0		29/2		29/2	19 809.94	.05	329
		15, 9, 6←15, 9, 7	Ground	A	0		33/2		33/2	19 818.39	.05	329
		15, 9, 6←15, 9, 7	Ground	A	0		27/2		27/2	19 819.38	.05	329
		15,10, 6←15, 8, 7	Ground	A	0		31/2		31/2	19 809.09	.05	329
		15,10, 6←15, 8, 7	Ground	A	0		29/2		29/2	19 809.94	.05	329
		15,10, 6←15, 8, 7	Ground	A	0		33/2		33/2	19 818.39	.05	329
		15,10, 6←15, 8, 7	Ground	A	0		27/2		27/2	19 819.38	.05	329
		16,10, 6←16,10, 7	Ground	A	0		33/2		33/2	19 804.60	.05	329
		16,10, 6←16,10, 7	Ground	A	0		31/2		31/2	19 805.38	.05	329
		16,10, 6←16,10, 7	Ground	A	0		35/2		35/2	19 812.87	.05	329
		16,10, 6←16,10, 7	Ground	A	0		29/2		29/2	19 813.68	.05	329
		16,11, 6←16, 9, 7	Ground	A	0		33/2		33/2	19 804.60	.05	329
		16,11, 6←16, 9, 7	Ground	A	0		31/2		31/2	19 805.38	.05	329
		16,11, 6←16, 9, 7	Ground	A	0		35/2		35/2	19 812.87	.05	329
		16,11, 6←16, 9, 7	Ground	A	0		29/2		29/2	19 813.68	.05	329
		16,11, 5←16,11, 6	Ground	A	0		33/2		33/2	16 745.69	.05	329
		16,11, 5←16,11, 6	Ground	A	0		31/2		31/2	16 746.44	.05	329
		16,11, 5←16,11, 6	Ground	A	0		35/2		35/2	16 753.14	.05	329
		16,11, 5←16,11, 6	Ground	A	0		29/2		29/2	16 753.84	.05	329
		16,12, 5←16,10, 6	Ground	A	0		33/2		33/2	16 745.69	.05	329
		16,12, 5←16,10, 6	Ground	A	0		31/2		31/2	16 746.44	.05	329
		16,12, 5←16,10, 6	Ground	A	0		35/2		35/2	16 753.14	.05	329
		16,12, 5←16,10, 6	Ground	A	0		29/2		29/2	16 753.84	.05	329
		16,12, 4←16,12, 5	Ground	A	0		33/2		33/2	13 673.03	.05	329
		16,12, 4←16,12, 5	Ground	A	0		31/2		31/2	13 673.74	.05	329
		16,12, 4←16,12, 5	Ground	E	0		33/2		33/2	13 677.04	.05	329
		16,12, 4←16,12, 5	Ground	E	0		31/2		31/2	13 677.67	.05	329
		16,12, 4←16,12, 5	Ground	A	0		35/2		35/2	13 679.95	.05	329
		16,12, 4←16,12, 5	Ground	A	0		29/2		29/2	13 680.63	.05	329
		16,12, 4←16,12, 5	Ground	E	0		35/2		35/2	13 683.88	.05	329
		16,12, 4←16,12, 5	Ground	E	0		29/2		29/2	13 684.50	.05	329
		16,13, 4←16,11, 5	Ground	E	0		33/2		33/2	13 674.34	.05	329
		16,13, 4←16,11, 5	Ground	E	0		31/2		31/2	13 675.04	.05	329
		16,13, 4←16,11, 5	Ground	A	0		33/2		33/2	13 678.73	.05	329
		16,13, 4←16,11, 5	Ground	A	0		31/2		31/2	13 679.34	.05	329
		16,13, 4←16,11, 5	Ground	E	0		35/2		35/2	13 681.13	.05	329
		16,13, 4←16,11, 5	Ground	E	0		29/2		29/2	13 681.72	.05	329
		16,13, 4←16,11, 5	Ground	A	0		35/2		35/2	13 685.30	.05	329
		16,13, 4←16,11, 5	Ground	A	0		29/2		29/2	13 685.89	.05	329
		17,11, 6←17,11, 7	Ground	A	0		35/2		35/2	19 799.25	.05	329
		17,11, 6←17,11, 7	Ground	A	0		37/2		37/2	19 806.78	.05	329
		17,11, 6←17,11, 7	Ground	A	0		31/2		31/2	19 807.40	.05	329
		17,12, 6←17,10, 7	Ground	A	0		35/2		35/2	19 799.25	.05	329
		17,12, 6←17,10, 7	Ground	A	0		37/2		37/2	19 806.78	.05	329
		17,12, 6←17,10, 7	Ground	A	0		31/2		31/2	19 807.40	.05	329
		17,12, 5←17,12, 6	Ground	A	0		35/2		35/2	16 738.29	.05	329
		17,12, 5←17,12, 6	Ground	A	0		33/2		33/2	16 738.84	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	17,12, 5←17,12, 6	Ground	E	0		35/2		35/2	16 739.50	.05	329
		17,12, 5←17,12, 6	Ground	E	0		33/2		33/2	16 740.00	.05	329
		17,12, 5←17,12, 6	Ground	E	0		37/2		37/2	16 742.70	.05	329
		17,12, 5←17,12, 6	Ground	E	0		31/2		31/2	16 743.13	.05	329
		17,12, 5←17,12, 6	Ground	A	0		37/2		37/2	16 745.03	.05	329
		17,12, 5←17,12, 6	Ground	A	0		31/2		31/2	16 745.69	.05	329
		17,13, 5←17,11, 6	Ground	A	0		35/2		35/2	16 738.29	.05	329
		17,13, 5←17,11, 6	Ground	A	0		33/2		33/2	16 738.84	.05	329
		17,13, 5←17,11, 6	Ground	E	0		35/2		35/2	16 739.50	.05	329
		17,13, 5←17,11, 6	Ground	E	0		33/2		33/2	16 740.00	.05	329
		17,13, 5←17,11, 6	Ground	E	0		37/2		37/2	16 742.70	.05	329
		17,13, 5←17,11, 6	Ground	E	0		31/2		31/2	16 743.13	.05	329
		17,13, 5←17,11, 6	Ground	A	0		37/2		37/2	16 745.03	.05	329
		17,13, 5←17,11, 6	Ground	A	0		31/2		31/2	16 745.69	.05	329
		17,13, 4←17,13, 5	Ground	A	0		35/2		35/2	13 658.73	.05	329
		17,13, 4←17,13, 5	Ground	A	0		33/2		33/2	13 659.24	.05	329
		17,13, 4←17,13, 5	Ground	E	0		35/2		35/2	13 663.71	.05	329
		17,13, 4←17,13, 5	Ground	E	0		33/2		33/2	13 664.28	.05	329
		17,13, 4←17,13, 5	Ground	A	0		37/2		37/2	13 665.24	.05	329
		17,13, 4←17,13, 5	Ground	A	0		31/2		31/2	13 665.81	.05	329
		17,13, 4←17,13, 5	Ground	E	0		37/2		37/2	13 670.12	.05	329
		17,13, 4←17,13, 5	Ground	E	0		31/2		31/2	13 670.61	.05	329
		17,14, 4←17,12, 5	Ground	E	0		35/2		35/2	13 662.75	.05	329
		17,14, 4←17,12, 5	Ground	E	0		33/2		33/2	13 663.27	.05	329
		17,14, 4←17,12, 5	Ground	A	0		35/2		35/2	13 667.71	.05	329
		17,14, 4←17,12, 5	Ground	A	0		33/2		33/2	13 668.23	.05	329
		17,14, 4←17,12, 5	Ground	E	0		37/2		37/2	13 668.90	.05	329
		17,14, 4←17,12, 5	Ground	E	0		31/2		31/2	13 669.39	.05	329
		17,14, 4←17,12, 5	Ground	A	0		37/2		37/2	13 673.74	.05	329
		17,14, 4←17,12, 5	Ground	A	0		31/2		31/2	13 674.34	.05	329
		18,13, 5←18,13, 6	Ground	E	0		37/2		37/2	16 727.30	.05	329
		18,13, 5←18,13, 6	Ground	E	0		35/2		35/2	16 727.80	.05	329
		18,13, 5←18,13, 6	Ground	E	0		37/2		37/2	16 730.71	.05	329
		18,13, 5←18,13, 6	Ground	E	0		35/2		35/2	16 731.22	.05	329
		18,13, 5←18,13, 6	Ground	E	0		39/2		39/2	16 733.47	.05	329
		18,13, 5←18,13, 6	Ground	E	0		33/2		33/2	16 733.96	.05	329
		18,13, 5←18,13, 6	Ground	E	0		39/2		39/2	16 736.85	.05	329
		18,13, 5←18,13, 6	Ground	E	0		33/2		33/2	16 737.38	.05	329
		18,14, 5←18,12, 6	Ground	E	0		37/2		37/2	16 727.30	.05	329
		18,14, 5←18,12, 6	Ground	E	0		35/2		35/2	16 727.80	.05	329
		18,14, 5←18,12, 6	Ground	E	0		37/2		37/2	16 730.71	.05	329
		18,14, 5←18,12, 6	Ground	E	0		35/2		35/2	16 731.22	.05	329
		18,14, 5←18,12, 6	Ground	E	0		39/2		39/2	16 733.47	.05	329
		18,14, 5←18,12, 6	Ground	E	0		33/2		33/2	16 733.96	.05	329
		18,14, 5←18,12, 6	Ground	E	0		39/2		39/2	16 736.85	.05	329
		18,14, 5←18,12, 6	Ground	E	0		33/2		33/2	16 737.38	.05	329
		18,14, 4←18,14, 5	Ground	A	0		37/2		37/2	13 641.15	.05	329
		18,14, 4←18,14, 5	Ground	A	0		35/2		35/2	13 641.60	.05	329
		18,14, 4←18,14, 5	Ground	A	0		39/2		39/2	13 647.31	.05	329
		18,14, 4←18,14, 5	Ground	E	0		37/2		37/2	13 647.31	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	18,14, 4←18,14, 5	Ground	A	0		33/2		33/2	13 647.79	.05	329
		18,14, 4←18,14, 5	Ground	E	0		35/2		35/2	13 647.79	.05	329
		18,14, 4←18,14, 5	Ground	E	0		39/2		39/2	13 653.49	.05	329
		18,14, 4←18,14, 5	Ground	E	0		33/2		33/2	13 653.97	.05	329
		18,15, 4←18,13, 5	Ground	E	0		37/2		37/2	13 649.58	.05	329
		18,15, 4←18,13, 5	Ground	E	0		35/2		35/2	13 650.09	.05	329
		18,15, 4←18,13, 5	Ground	A	0		37/2		37/2	13 655.27	.05	329
		18,15, 4←18,13, 5	Ground	E	0		39/2		39/2	13 655.27	.05	329
		18,15, 4←18,13, 5	Ground	A	0		35/2		35/2	13 655.68	.05	329
		18,15, 4←18,13, 5	Ground	E	0		33/2		33/2	13 655.68	.05	329
		18,15, 4←18,13, 5	Ground	A	0		39/2		39/2	13 660.85	.05	329
		18,15, 4←18,13, 5	Ground	A	0		33/2		33/2	13 661.24	.05	329
		19,14, 5←19,14, 6	Ground	A	0		39/2		39/2	16 719.06	.05	329
		19,14, 5←19,14, 6	Ground	A	0		37/2		37/2	16 719.53	.05	329
		19,14, 5←19,14, 6	Ground	E	0		39/2		39/2	16 720.59	.05	329
		19,14, 5←19,14, 6	Ground	E	0		37/2		37/2	16 721.05	.05	329
		19,14, 5←19,14, 6	Ground	A	0		41/2		41/2	16 724.80	.05	329
		19,14, 5←19,14, 6	Ground	A	0		35/2		35/2	16 725.24	.05	329
		19,14, 5←19,14, 6	Ground	E	0		41/2		41/2	16 726.29	.05	329
		19,14, 5←19,14, 6	Ground	E	0		35/2		35/2	16 726.71	.05	329
		19,15, 5←19,13, 6	Ground	E	0		39/2		39/2	16 717.31	.05	329
		19,15, 5←19,13, 6	Ground	E	0		37/2		37/2	16 717.75	.05	329
		19,15, 5←19,13, 6	Ground	A	0		39/2		39/2	16 719.53	.05	329
		19,15, 5←19,13, 6	Ground	A	0		37/2		37/2	16 719.98	.05	329
		19,15, 5←19,13, 6	Ground	E	0		41/2		41/2	16 723.04	.05	329
		19,15, 5←19,13, 6	Ground	E	0		35/2		35/2	16 723.52	.05	329
		19,15, 5←19,13, 6	Ground	A	0		41/2		41/2	16 725.24	.05	329
		19,15, 5←19,13, 6	Ground	A	0		35/2		35/2	16 725.70	.05	329
		20,14, 6←20,14, 7	Ground	A	0		41/2		41/2	19 777.80	.05	329
		20,14, 6←20,14, 7	Ground	A	0		39/2		39/2	19 778.22	.05	329
		20,14, 6←20,14, 7	Ground	A	0		43/2		43/2	19 783.53	.05	329
		20,14, 6←20,14, 7	Ground	A	0		37/2		37/2	19 783.93	.05	329
		20,15, 6←20,13, 7	Ground	A	0		41/2		41/2	19 777.80	.05	329
		20,15, 6←20,13, 7	Ground	A	0		39/2		39/2	19 778.22	.05	329
		20,15, 6←20,13, 7	Ground	A	0		43/2		43/2	19 783.53	.05	329
		20,15, 6←20,13, 7	Ground	A	0		37/2		37/2	19 783.93	.05	329
		20,15, 5←20,15, 6	Ground	A	0		41/2		41/2	16 707.06	.05	329
		20,15, 5←20,15, 6	Ground	A	0		39/2		39/2	16 707.45	.05	329
		20,15, 5←20,15, 6	Ground	E	0		41/2		41/2	16 708.90	.05	329
		20,15, 5←20,15, 6	Ground	E	0		39/2		39/2	16 709.30	.05	329
		20,15, 5←20,15, 6	Ground	A	0		43/2		43/2	16 712.50	.05	329
		20,15, 5←20,15, 6	Ground	A	0		37/2		37/2	16 712.76	.05	329
		20,15, 5←20,15, 6	Ground	E	0		43/2		43/2	16 714.30	.05	329
		20,15, 5←20,15, 6	Ground	E	0		37/2		37/2	16 714.65	.05	329
		20,16, 5←20,14, 6	Ground	E	0		41/2		41/2	16 705.82	.05	329
		20,16, 5←20,14, 6	Ground	E	0		39/2		39/2	16 706.22	.05	329
		20,16, 5←20,14, 6	Ground	A	0		41/2		41/2	16 708.04	.05	329
		20,16, 5←20,14, 6	Ground	A	0		39/2		39/2	16 708.44	.05	329
		20,16, 5←20,14, 6	Ground	E	0		43/2		43/2	16 711.15	.05	329
		20,16, 5←20,14, 6	Ground	E	0		37/2		37/2	16 711.55	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	20,16, 5←20,14, 6	Ground	A	0		43/2		43/2	16 713.39	.05	329
		20,16, 5←20,14, 6	Ground	A	0		37/2		37/2	16 713.73	.05	329
		21,15, 6←21,15, 7	Ground	A	0		43/2		43/2	19 768.51	.05	329
		21,15, 6←21,15, 7	Ground	A	0		41/2		41/2	19 768.95	.05	329
		21,15, 6←21,15, 7	Ground	A	0		45/2		45/2	19 773.93	.05	329
		21,15, 6←21,15, 7	Ground	A	0		39/2		39/2	19 774.22	.05	329
		21,16, 6←21,14, 7	Ground	A	0		43/2		43/2	19 768.51	.05	329
		21,16, 6←21,14, 7	Ground	A	0		41/2		41/2	19 768.95	.05	329
		21,16, 6←21,14, 7	Ground	A	0		45/2		45/2	19 773.93	.05	329
		21,16, 6←21,14, 7	Ground	A	0		39/2		39/2	19 774.22	.05	329
		22,16, 6←22,16, 7	Ground	E	0		45/2		45/2	19 756.43	.05	329
		22,16, 6←22,16, 7	Ground	A	0		43/2		43/2	19 758.40	.05	329
		22,16, 6←22,16, 7	Ground	A	0		45/2		45/2	19 758.40	.05	329
		22,16, 6←22,16, 7	Ground	E	0		43/2		43/2	19 759.34	.05	329
		22,16, 6←22,16, 7	Ground	E	0		41/2		41/2	19 761.35	.05	329
		22,16, 6←22,16, 7	Ground	A	0		47/2		47/2	19 763.34	.05	329
		22,16, 6←22,16, 7	Ground	A	0		41/2		41/2	19 763.34	.05	329
		22,16, 6←22,16, 7	Ground	E	0		47/2		47/2	19 764.30	.05	329
		22,17, 6←22,15, 7	Ground	E	0		45/2		45/2	19 756.43	.05	329
		22,17, 6←22,15, 7	Ground	A	0		43/2		43/2	19 758.40	.05	329
		22,17, 6←22,15, 7	Ground	A	0		45/2		45/2	19 758.40	.05	329
		22,17, 6←22,15, 7	Ground	E	0		43/2		43/2	19 759.34	.05	329
		22,17, 6←22,15, 7	Ground				43/2		43/2	19 759.34	.05	329
		22,17, 6←22,15, 7	Ground	E	0		41/2		41/2	19 761.35	.05	329
		22,17, 6←22,15, 7	Ground	A	0		47/2		47/2	19 763.34	.05	329
		22,17, 6←22,15, 7	Ground	A	0		41/2		41/2	19 763.34	.05	329
		22,17, 6←22,15, 7	Ground	E	0		47/2		47/2	19 764.30	.05	329
		22,17, 6←22,15, 7	Ground				47/2		47/2	19 764.30	.05	329
		22,17, 5←22,17, 6	Ground	E	0		45/2		45/2	16 680.39	.05	329
		22,17, 5←22,17, 6	Ground	E	0		43/2		43/2	16 680.63	.05	329
		22,17, 5←22,17, 6	Ground	A	0		47/2		47/2	16 682.54	.05	329
		22,17, 5←22,17, 6	Ground	A	0		41/2		41/2	16 682.87	.05	329
		22,17, 5←22,17, 6	Ground	E	0		47/2		47/2	16 685.19	.05	329
		22,17, 5←22,17, 6	Ground	E	0		41/2		41/2	16 685.46	.05	329
		22,18, 5←22,16, 6	Ground	A	0		45/2		45/2	16 680.13	.05	329
		22,18, 5←22,16, 6	Ground	A	0		43/2		43/2	16 680.39	.05	329
		22,18, 5←22,16, 6	Ground	E	0		47/2		47/2	16 682.54	.05	329
		22,18, 5←22,16, 6	Ground	E	0		41/2		41/2	16 682.87	.05	329
		22,18, 5←22,16, 6	Ground	A	0		47/2		47/2	16 684.93	.05	329
		22,18, 5←22,16, 6	Ground	A	0		41/2		41/2	16 685.19	.05	329
		23,17, 6←23,17, 7	Ground	E	0		47/2		47/2	19 745.16	.05	329
		23,17, 6←23,17, 7	Ground	A	0		45/2		45/2	19 746.89	.05	329
		23,17, 6←23,17, 7	Ground	A	0		47/2		47/2	19 746.89	.05	329
		23,17, 6←23,17, 7	Ground	E	0		45/2		45/2	19 747.82	.05	329
		23,17, 6←23,17, 7	Ground	E	0		43/2		43/2	19 749.81	.05	329
		23,17, 6←23,17, 7	Ground	A	0		49/2		49/2	19 751.49	.05	329
		23,17, 6←23,17, 7	Ground	A	0		43/2		43/2	19 751.49	.05	329
		23,17, 6←23,17, 7	Ground	E	0		49/2		49/2	19 752.44	.05	329
		23,18, 6←23,16, 7	Ground	E	0		47/2		47/2	19 745.16	.05	329
		23,18, 6←23,16, 7	Ground	A	0		45/2		45/2	19 746.89	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	23,18, 6←23,16, 7	Ground	A	0		47/2		47/2	19 746.89	.05	329
		23,18, 6←23,16, 7	Ground	E	0		45/2		45/2	19 747.82	.05	329
		23,18, 6←23,16, 7	Ground	E	0		43/2		43/2	19 749.81	.05	329
		23,18, 6←23,16, 7	Ground	A	0		49/2		49/2	19 751.49	.05	329
		23,18, 6←23,16, 7	Ground	A	0		43/2		43/2	19 751.49	.05	329
		23,18, 6←23,16, 7	Ground	E	0		49/2		49/2	19 752.44	.05	329
		23,18, 5←23,18, 6	Ground	A	0		47/2		47/2	16 659.49	.05	329
		23,18, 5←23,18, 6	Ground	A	0		45/2		45/2	16 659.86	.05	329
		23,18, 5←23,18, 6	Ground	E	0		47/2		47/2	16 663.09	.05	329
		23,18, 5←23,18, 6	Ground	E	0		45/2		45/2	16 663.35	.05	329
		23,18, 5←23,18, 6	Ground	A	0		49/2		49/2	16 664.29	.05	329
		23,18, 5←23,18, 6	Ground	A	0		43/2		43/2	16 664.56	.05	329
		23,18, 5←23,18, 6	Ground	E	0		49/2		49/2	16 667.74	.05	329
		23,18, 5←23,18, 6	Ground	E	0		43/2		43/2	16 667.99	.05	329
		23,19, 5←23,17, 6	Ground	E	0		47/2		47/2	16 660.96	.05	329
		23,19, 5←23,17, 6	Ground	E	0		45/2		45/2	16 661.14	.05	329
		23,19, 5←23,17, 6	Ground	A	0		45/2		45/2	16 663.76	.05	329
		23,19, 5←23,17, 6	Ground	E	0		49/2		49/2	16 665.55	.05	329
		23,19, 5←23,17, 6	Ground	E	0		43/2		43/2	16 665.82	.05	329
		23,19, 5←23,17, 6	Ground	A	0		49/2		49/2	16 667.99	.05	329
		23,19, 5←23,17, 6	Ground	A	0		43/2		43/2	16 668.31	.05	329
		24,18, 6←24,18, 7	Ground	E	0		49/2		49/2	19 732.30	.05	329
		24,18, 6←24,18, 7	Ground	A	0		47/2		47/2	19 733.79	.05	329
		24,18, 6←24,18, 7	Ground	A	0		49/2		49/2	19 733.79	.05	329
		24,18, 6←24,18, 7	Ground	E	0		47/2		47/2	19 734.90	.05	329
		24,18, 6←24,18, 7	Ground	E	0		45/2		45/2	19 736.79	.05	329
		24,18, 6←24,18, 7	Ground	A	0		51/2		51/2	19 738.29	.05	329
		24,18, 6←24,18, 7	Ground	A	0		45/2		45/2	19 738.29	.05	329
		24,18, 6←24,18, 7	Ground	E	0		51/2		51/2	19 739.39	.05	329
		24,19, 6←24,17, 7	Ground	E	0		49/2		49/2	19 732.30	.05	329
		24,19, 6←24,17, 7	Ground	A	0		47/2		47/2	19 733.79	.05	329
		24,19, 6←24,17, 7	Ground	A	0		49/2		49/2	19 733.79	.05	329
		24,19, 6←24,17, 7	Ground	E	0		47/2		47/2	19 734.90	.05	329
		24,19, 6←24,17, 7	Ground	E	0		45/2		45/2	19 736.79	.05	329
		24,19, 6←24,17, 7	Ground	A	0		51/2		51/2	19 738.29	.05	329
		24,19, 6←24,17, 7	Ground	A	0		45/2		45/2	19 738.29	.05	329
		24,19, 6←24,17, 7	Ground	E	0		51/2		51/2	19 739.39	.05	329
		24,19, 5←24,19, 6	Ground	A	0		49/2		49/2	16 639.06	.05	329
		24,19, 5←24,19, 6	Ground	A	0		47/2		47/2	16 639.36	.05	329
		24,19, 5←24,19, 6	Ground	E	0		51/2		51/2	16 647.94	.05	329
		24,19, 5←24,19, 6	Ground	E	0		45/2		45/2	16 648.05	.05	329
		24,20, 5←24,18, 6	Ground	E	0		49/2		49/2	16 642.15	.05	329
		24,20, 5←24,18, 6	Ground	E	0		47/2		47/2	16 642.38	.05	329
		24,20, 5←24,18, 6	Ground	A	0		49/2		49/2	16 644.97	.05	329
		24,20, 5←24,18, 6	Ground	A	0		47/2		47/2	16 645.19	.05	329
		24,20, 5←24,18, 6	Ground	E	0		51/2		51/2	16 646.57	.05	329
		24,20, 5←24,18, 6	Ground	E	0		45/2		45/2	16 646.82	.05	329
		24,20, 5←24,18, 6	Ground	A	0		51/2		51/2	16 649.41	.05	329
		24,20, 5←24,18, 6	Ground	A	0		45/2		45/2	16 649.63	.05	329
		25,19, 6←25,19, 7	Ground	E	0		51/2		51/2	19 718.14	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	25,19, 6←25,19, 7	Ground	A	0		49/2		49/2	19 719.24	.05	329
		25,19, 6←25,19, 7	Ground	A	0		51/2		51/2	19 719.24	.05	329
		25,19, 6←25,19, 7	Ground	E	0		49/2		49/2	19 720.54	.05	329
		25,19, 6←25,19, 7	Ground	E	0		47/2		47/2	19 722.36	.05	329
		25,19, 6←25,19, 7	Ground	A	0		53/2		53/2	19 723.46	.05	329
		25,19, 6←25,19, 7	Ground	A	0		47/2		47/2	19 723.46	.05	329
		25,19, 6←25,19, 7	Ground	E	0		53/2		53/2	19 724.74	.05	329
		25,20, 6←25,18, 7	Ground	E	0		51/2		51/2	19 718.14	.05	329
		25,20, 6←25,18, 7	Ground	A	0		49/2		49/2	19 719.24	.05	329
		25,20, 6←25,18, 7	Ground	A	0		51/2		51/2	19 719.24	.05	329
		25,20, 6←25,18, 7	Ground	E	0		49/2		49/2	19 720.54	.05	329
		25,20, 6←25,18, 7	Ground	E	0		47/2		47/2	19 722.36	.05	329
		25,20, 6←25,18, 7	Ground	A	0		47/2		47/2	19 723.46	.05	329
		25,20, 6←25,18, 7	Ground	E	0		53/2		53/2	19 724.74	.05	329
		25,20, 5←25,20, 6	Ground	A	0		51/2		51/2	16 615.68	.05	329
		25,20, 5←25,20, 6	Ground	A	0		49/2		49/2	16 615.92	.05	329
		25,20, 5←25,20, 6	Ground	A	0		53/2		53/2	16 620.20	.05	329
		25,20, 5←25,20, 6	Ground	A	0		47/2		47/2	16 620.45	.05	329
		25,20, 5←25,20, 6	Ground	E	0		51/2		51/2	16 620.96	.05	329
		25,20, 5←25,20, 6	Ground	E	0		49/2		49/2	16 621.21	.05	329
		25,20, 5←25,20, 6	Ground	E	0		53/2		53/2	16 625.44	.05	329
		25,20, 5←25,20, 6	Ground	E	0		47/2		47/2	16 625.75	.05	329
		25,21, 5←25,19, 6	Ground	E	0		51/2		51/2	16 621.38	.05	329
		25,21, 5←25,19, 6	Ground	E	0		49/2		49/2	16 621.61	.05	329
		25,21, 5←25,19, 6	Ground	A	0		51/2		51/2	16 624.54	.05	329
		25,21, 5←25,19, 6	Ground	A	0		49/2		49/2	16 624.78	.05	329
		25,21, 5←25,19, 6	Ground	E	0		53/2		53/2	16 625.44	.05	329
		25,21, 5←25,19, 6	Ground	E	0		47/2		47/2	16 625.75	.05	329
		25,21, 5←25,19, 6	Ground	A	0		53/2		53/2	16 628.81	.05	329
		25,21, 5←25,19, 6	Ground	A	0		47/2		47/2	16 629.05	.05	329
		26,20, 6←26,20, 7	Ground	E	0		53/2		53/2	19 702.69	.05	329
		26,20, 6←26,20, 7	Ground	A	0		51/2		51/2	19 703.62	.05	329
		26,20, 6←26,20, 7	Ground	A	0		53/2		53/2	19 703.62	.05	329
		26,20, 6←26,20, 7	Ground	E	0		51/2		51/2	19 704.87	.05	329
		26,20, 6←26,20, 7	Ground	E	0		49/2		49/2	19 706.70	.05	329
		26,20, 6←26,20, 7	Ground	A	0		55/2		55/2	19 707.62	.05	329
		26,20, 6←26,20, 7	Ground	A	0		49/2		49/2	19 707.62	.05	329
		26,20, 6←26,20, 7	Ground	E	0		55/2		55/2	19 708.87	.05	329
		26,21, 6←26,19, 7	Ground	E	0		53/2		53/2	19 702.69	.05	329
		26,21, 6←26,19, 7	Ground	A	0		51/2		51/2	19 703.62	.05	329
		26,21, 6←26,19, 7	Ground	A	0		53/2		53/2	19 703.62	.05	329
		26,21, 6←26,19, 7	Ground	E	0		51/2		51/2	19 704.87	.05	329
		26,21, 6←26,19, 7	Ground	E	0		49/2		49/2	19 706.70	.05	329
		26,21, 6←26,19, 7	Ground	A	0		55/2		55/2	19 707.62	.05	329
		26,21, 6←26,19, 7	Ground	A	0		49/2		49/2	19 707.62	.05	329
		26,21, 6←26,19, 7	Ground	E	0		55/2		55/2	19 708.87	.05	329
		26,21, 5←26,21, 6	Ground	A	0		53/2		53/2	16 589.19	.05	329
		26,21, 5←26,21, 6	Ground	A	0		51/2		51/2	16 589.19	.05	329
		26,21, 5←26,21, 6	Ground	A	0		55/2		55/2	16 593.72	.05	329
		26,21, 5←26,21, 6	Ground	A	0		49/2		49/2	16 593.72	.05	329

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3As^{75}F_2^{19}$	81	26,21, 5←26,21, 6	Ground	E	0		53/2		53/2	16 595.32	.05	329
		26,21, 5←26,21, 6	Ground	E	0		51/2		51/2	16 595.32	.05	329
		26,21, 5←26,21, 6	Ground	E	0		55/2		55/2	16 599.81	.05	329
		26,21, 5←26,21, 6	Ground	E	0		49/2		49/2	16 599.81	.05	329
		26,22, 5←26,20, 6	Ground	E	0		53/2		53/2	16 598.89	.05	329
		26,22, 5←26,20, 6	Ground	E	0		51/2		51/2	16 598.89	.05	329
		26,22, 5←26,20, 6	Ground	A	0		53/2		53/2	16 602.22	.05	329
		26,22, 5←26,20, 6	Ground	A	0		51/2		51/2	16 602.22	.05	329
		26,22, 5←26,20, 6	Ground	E	0		55/2		55/2	16 602.97	.05	329
		26,22, 5←26,20, 6	Ground	E	0		49/2		49/2	16 602.97	.05	329
		26,22, 5←26,20, 6	Ground	A	0		55/2		55/2	16 606.36	.05	329
		26,22, 5←26,20, 6	Ground	A	0		49/2		49/2	16 606.36	.05	329
		27,22, 5←27,22, 6	Ground	A	0		55/2		55/2	16 558.95	.05	329
		27,22, 5←27,22, 6	Ground	A	0		53/2		53/2	16 558.95	.05	329
		27,22, 5←27,22, 6	Ground	A	0		57/2		57/2	16 563.55	.05	329
		27,22, 5←27,22, 6	Ground	A	0		51/2		51/2	16 563.55	.05	329
		27,22, 5←27,22, 6	Ground	E	0		55/2		55/2	16 565.86	.05	329
		27,22, 5←27,22, 6	Ground	E	0		53/2		53/2	16 565.86	.05	329
		27,22, 5←27,22, 6	Ground	E	0		57/2		57/2	16 570.36	.05	329
		27,22, 5←27,22, 6	Ground	E	0		51/2		51/2	16 570.36	.05	329
		27,23, 5←27,21, 6	Ground	E	0		55/2		55/2	16 574.40	.05	329
		27,23, 5←27,21, 6	Ground	E	0		53/2		53/2	16 574.40	.05	329
		27,23, 5←27,21, 6	Ground	A	0		55/2		55/2	16 577.85	.05	329
		27,23, 5←27,21, 6	Ground	A	0		53/2		53/2	16 577.85	.05	329
		27,23, 5←27,21, 6	Ground	E	0		57/2		57/2	16 578.40	.05	329
		27,23, 5←27,21, 6	Ground	E	0		51/2		51/2	16 578.40	.05	329
		27,23, 5←27,21, 6	Ground	A	0		57/2		57/2	16 581.88	.05	329
		27,23, 5←27,21, 6	Ground	A	0		51/2		51/2	16 581.88	.05	329
		28,23, 5←28,23, 6	Ground	A	0		57/2		57/2	16 524.58	.05	329
		28,23, 5←28,23, 6	Ground	A	0		55/2		55/2	16 524.58	.05	329
		28,23, 5←28,23, 6	Ground	A	0		59/2		59/2	16 529.17	.05	329
		28,23, 5←28,23, 6	Ground	A	0		53/2		53/2	16 529.17	.05	329
		28,24, 5←28,22, 6	Ground	A	0		57/2		57/2	16 551.39	.05	329
		28,24, 5←28,22, 6	Ground	A	0		55/2		55/2	16 551.39	.05	329
		28,24, 5←28,22, 6	Ground	A	0		59/2		59/2	16 555.31	.05	329
		28,24, 5←28,22, 6	Ground	A	0		53/2		53/2	16 555.31	.05	329

CH_3BF_2 $C_s(C_{3v},C_{2v})$ CH_3BF_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3B^bF_2^{19}$	C_s	91		8 329.01 M	4 650.52 M				0.257

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_6	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
91	1.67 M		0. X		13.77	.03					

References:

ABC: 186 D_J: D_{JK}: κ: Δ: 116

μ: 186 eQq: V: 186 I: ω:

Add. Refs.: 125, 195

Rotational constant for BF_2 group only: A = 10586.73 MHz. Ref: 186.

Methyldifluoroborane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3B^bF_2^{19}$	91	1, , ← 0, ,	Ground	e0					12 979.4	.1	186
		2, , ← 1, ,	Ground	e0					3 773.5	.1	186
		2, , ← 1, ,	Ground	o0					22 280.6	.1	186
		2, , ← 1, ,	Ground	o3					23 999.7	.1	186
		2, , ← 1, ,	Ground	o3					24 278.8	.1	186
		2, , ← 1, ,	Ground	o2					25 635.5	.1	186
		2, , ← 1, ,	Ground	e3					25 817.4	.1	186
		2, , ← 1, ,	Ground	e2					26 054.3	.1	186
		2, , ← 1, ,	Ground	e3					26 201.6	.1	186
		2, , ← 1, ,	Ground	o2					26 276.7	.1	186
		2, , ← 1, ,	Ground	o1					26 590.5	.1	186
		2, , ← 1, ,	Ground	o3					27 625.8	.1	186
		2, , ← 1, ,	Ground	o3					27 904.3	.1	186
		2, , ← 1, ,	Ground	o0					29 637.6	.1	186
		3, , ← 2, ,	Ground	o0					32 291.8	.1	186
		4, , ← 4, ,	Ground	o0					31 575.1	.1	186
		6, , ← 6, ,	Ground	o0					25 107.2	.1	186
		9, , ← 9, ,	Ground	o0					26 548.0	.1	186
		12, , ←12, ,	Ground	o0					25 848.0	.1	186

CH_3Cl_3Ge $C_{3v}(C_{3v},C_{3v})$ CH_3GeCl_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Ge^{70}Cl_3^{35}$	C_{3v}	101							
$C^{12}H_3Ge^{74}Cl_2^{35}Cl^{37}$	C_s	106	1 585. M	1 567. M	1 192. M				
$C^{12}H_3Ge^{b}Cl_3^{35}$	C_{3v}	107	1 599.3 M	1 599.3 M					

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
101	0. X	0. X	2.63 [1] M								

1. Value recorded was for compound in benzene solution, no gas determination being available.

References:

ABC: 216, 217 D_J: D_{JK}: κ: Δ:

μ: 382 eQq: V: I: ω:

Methyltrichlorogermane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Ge^{b}Cl^{35}Cl_2^{37}$	104	3, 2, 2← 2, 1, 2							9 315.	15.	216
		5, 2, 4← 4, 1, 4							15 530.	15.	216
		6, 2, 6← 5, 1, 4							18 665.	15.	216
$C^{12}H_3Ge^{b}Cl_2^{35}Cl^{37}$	105	3, 2, 2← 2, 1, 2							9 455.	15.	216
		5, 2, 4← 4, 1, 4							15 755.	15.	216
		6, 2, 6← 5, 1, 4							18 910.	15.	216
		8, 3, 6← 7, 2, 6							25 220.	15.	216
$C^{12}H_3Ge^{b}Cl_3^{35}$	107	3, ← 2,							9 595.	15.	217
		5, ← 4,							15 995.	15.	217
		6, ← 5,							19 190.	15.	217
		8, ← 7,							25 590.	15.	217

110 - Methyltrichlorosilane
Methyltrichlorosilicane

Molecular Constant Table

CH_3Cl_3Si $C_{3v}(C_{3v},C_{3v})$ ClH_3SiCl_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Si^{28}Cl_3^{35}$	C_{3v}	111	1 769.836 M	1 769.836 M	1 317. M		<.010		
$C^{12}H_3Si^{28}Cl_3^{37}$	C_{3v}	112	1 699.791 M	1 699.791 M					

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
111	0. X	0. X	1.93[1] L								

1. Benzene solution determination of dipole moment is value given; no gas determination value was available.

References:

ABC: 79, 303 D_J: D_{JK}: 79 κ: Δ:

μ: 364 eQq: V: I: ω:

Add. Ref.: 58, 85

Methyltrichlorosilane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Si^{28}Cl_3^{35}$	111	9, ← 8,							31 840.	20.	79
		10. ← 9,	Excited						35 396.71	.5	79
		11, ←10,							38 950.	20.	79
		12, ←11,							42 500.	25.	79
$C^{12}H_3Si^{28}Cl_3^{37}$	112	9, ← 8,	Excited						30 569.09	.5	79
		10, ← 9,	Excited						33 995.81	.5	79
$C^{12}H_3Si^{28}Cl_2^{35}Cl^{37}$	113	9, , ← 8, ,							31 410.	10.	79
		10, , ← 9, ,	Excited						34 902.3	.5	79
		11, , ←10, ,							38 400.	10.	79
		12, , ←11, ,							41 900.	20.	79
$C^{12}H_3Si^{28}Cl^{35}Cl_2^{37}$	114	9, , ← 8, ,	Ground						30 980.	20.	79
		10, , ← 9, ,	Ground						34 400.	20.	79
		11, , ←10, ,	Ground						37 900.	20.	79
		12, , ←11, ,	Ground						41 310.	20.	79

120 - Methyltrifluorogermane[1] Molecular Constant Table

CH_3F_3Ge $C_{3v}(C_{3v},C_{3v})$ CH_3GeF_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Ge^bF_3^{19}$	C_{3v}	121		3 257. M	3 257. M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
121	3.8 M	0. X	0. X								

1. Absorption spectrum in the 10–30 kMHz range has been observed and records obtained for lines corresponding to transitions J=2←1,3←2,4←3, for both ground and excited states of internal rotation. However, these have not been reported in available literature.

References:

ABC: 387 D_J: D_{JK}: κ: Δ:

μ: 387 eQq: V: I: ω:

No spectral lines

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130 - Methyltrifluorosilane
Methyltrifluorosilicane Molecular Constant Table

CH_3F_3Si $C_{3v}(C_{3v},C_{3v})$ CH_3SiF_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Si^{28}F_3^{19}$	C_{3v}	131		3 715.66 M	3 715.66 M	.001	<.003		
$C^{12}D_3Si^{28}F_3^{19}$	C_{3v}	132		3 314.56 M	3 314.56 M				
$C^{13}D_3Si^{28}F_3^{19}$	C_{3v}	133		3 245.84 M	3 245.84 M				
$C^{12}H_2DSi^{28}F_3^{19}$	C_s	134	4 007. M	3 574.15 M	3 556.00 M				
$C^{12}HD_2Si^{28}F_3^{19}$	C_s	135	4 011. M	3 448.23 M	3 418.60 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
131	2.483 M	0. X	0. X		1200						

References:

ABC: 194, 303 D_J: 136 D_{JK}: 136 κ: Δ:

μ: 95 eQq: V: 48 I: ω:

Add. Refs.: 29, 43, 130, 374

Torsional frequency 141 cm^{-1}. Ref: 43.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Si^{28}F_3^{19}$	131	3, ← 2,	Excited						22 242.1		136
		3, ← 2,	Excited						22 244.4		136
		3, ← 2,	Excited						22 267.48		136
		3, ← 2,	Excited						22 278.47		136
		3, ← 2,	Ground						22 293.87	.1	136
		3, ← 2,	Excited						22 296.97		136
		3, ← 2,	Excited						22 323.32		136
		4, ← 3,	Excited						29 656.06		136
		4, ← 3,	Excited						29 659.06		136
		4, ← 3,	Excited						29 689.70		48
		4, ← 3,	Excited						29 690.07		48
		4, ← 3,	Excited						29 704.12		48
		4, ← 3,	Excited						29 704.70		48
		4, ← 3,	Excited						29 724.87		48
		4, ← 3,	Ground						29 724.99	.1	136
		4, ← 3,	Excited						29 729.13		136
		4, ← 3,	Excited						29 764.24		136
		5, ← 4,	Excited						37 025.7		136
		5, ← 4,	Excited						37 034.4		136
		5, ← 4,	Excited						37 046.5		136
		5, ← 4,	Excited						37 069.91		136
		5, ← 4,	Excited						37 073.67		136
		5, ← 4,	Excited						37 082.2		136
		5, ← 4,	Excited						37 112.05		136
		5, ← 4,	Excited						37 112.32		136
		5, ← 4,	Excited						37 129.86		136
		5, ← 4,	Excited						37 129.98		136
		5, ← 4,	Ground						37 156.07	.1	136
		5, ← 4,	Excited						37 161.16		136
		5, ← 4,	Excited						37 205.16		136
$C^{12}D_3Si^{28}F_3^{19}$	132	4, ← 3,	Excited						26 440.62		136
		4, ← 3,	Excited						26 463.93		136
		4, ← 3,	Excited						26 488.90		136
		4, ← 3,	Ground						26 516.20	.1	136
		4, ← 3,	Excited						26 545.72		136
		5, ← 4,	Excited						32 975.4		136
		5, ← 4,	Excited						32 999.3		136
		5, ← 4,	Excited						33 006.1		136
		5, ← 4,	Excited						33 022.6		136
		5, ← 4,	Excited						33 026.2		136
		5, ← 4,	Excited						33 032.3		136
		5, ← 4,	Excited						33 050.53		136
		5, ← 4,	Excited						33 052.04		136
		5, ← 4,	Excited						33 063.5		136
		5, ← 4,	Excited						33 079.78		136
		5, ← 4,	Excited						33 095.30		136
		5, ← 4,	Excited						33 110.97		136
		5, ← 4,	Excited						33 132.71		136
		5, ← 4,	Ground						33 145.02	.1	136
		5, ← 4,	Excited						33 148.51		136
		5, ← 4,	Excited						33 181.81		136

CH_3NO $C_s(C_s,C_s)$ CH_2NOH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_2N^{14}O^{16}H$	C_s	141	67 678.28 M	11 859.25 M	10 080.07 M				
$C^{12}H_2N^{14}O^{16}D$	C_s	142	66 167.74 M	11 081.66 M	9 484.57 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
141	0.397 M	0.18 M	0. X	3.0							
142				3.1							

References:

ABC: 295 D_J: D_{JK}: κ: Δ:

μ: 295, 354 eQq: 295 V: I: ω:

Add. Refs.: 348, 354, 376

For the first excited torsional state, the rotational constants for species 141 are: A = 66633.02 MHz, B = 11829.56 MHz, and C = 10087.99 MHz; anf for species 142 are: A = 64950.82 MHz, B = 11061.53 MHz, and C = 9503.03 MHz. The torsional frequency for species 141 is 330 ± 30 cm^{-1}. Ref: 295.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2N^{14}O^{16}H$	141	1, 0, 1← 0, 0, 0	Ground	1		0		1	21 916.06	.10	295
		1, 0, 1← 0, 0, 0	Ground	1		2		1	21 917.40	.10	295
		1, 0, 1← 0, 0, 0	Ground	1		1		1	21 918.33	.10	295
		1, 0, 1← 0, 0, 0	Ground			0		1	21 937.80	.10	295
		1, 0, 1← 0, 0, 0	Ground			2		1	21 939.17	.10	295
		1, 0, 1← 0, 0, 0	Ground			1		1	21 940.06	.10	295
		1, 1, 1← 2, 0, 2	Ground	1		1		2	11 007.38	.10	295
		1, 1, 1← 2, 0, 2	Ground	1		2		2	11 008.88	.10	295
		1, 1, 1← 2, 0, 2	Ground	1		1		1	11 008.88	.10	295
		1, 1, 1← 2, 0, 2	Ground	1		2		3	11 009.65	.10	295
		1, 1, 1← 2, 0, 2	Ground	1		0		1	11 012.32	.10	295
		1, 1, 1← 2, 0, 2	Ground			1		2	11 980.31	.10	295
		1, 1, 1← 2, 0, 2	Ground			2		2	11 981.85	.10	295
		1, 1, 1← 2, 0, 2	Ground			1		1	11 981.85	.10	295
		1, 1, 1← 2, 0, 2	Ground			2		3	11 982.69	.10	295
		1, 1, 1← 2, 0, 2	Ground			0		1	11 985.43	.10	295
		2, 0, 2← 1, 0, 1	Ground	1		3		2	43 794.02	.10	295
		2, 0, 2← 1, 0, 1	Ground	1		2		1	43 794.02	.10	295
		2, 0, 2← 1, 0, 1	Ground			3		2	43 836.50	.10	295
		2, 0, 2← 1, 0, 1	Ground			2		1	43 836.50	.10	295
		2, 0, 2← 1, 0, 1	Ground			2		2	43 837.38	.10	295
		2, 0, 2← 1, 0, 1	Ground			1		0	43 837.38	.10	295
		2, 1, 1← 1, 1, 0	Ground			1		0	45 657.30	.10	295
		2, 1, 1← 1, 1, 0	Ground			3		2	45 657.30	.10	295
		2, 1, 1← 1, 1, 0	Ground			2		1	45 658.40	.10	295
		2, 1, 2← 1, 1, 1	Ground	1		3		2	42 093.42	.10	295
		2, 1, 2← 1, 1, 1	Ground			1		0	42 097.58	.10	295
		2, 1, 2← 1, 1, 1	Ground			3		2	42 099.35	.10	295
		2, 1, 2← 1, 1, 1	Ground			2		1	42 100.24	.10	295
		2, 1, 1← 2, 0, 2	Ground			2		2	59 418.76	.10	295
		2, 1, 1← 2, 0, 2	Ground			3		3	59 418.76	.10	295
		2, 1, 1← 2, 0, 2	Ground			1		1	59 418.76	.10	295
		3, 0, 3← 2, 1, 2	Ground			2		1	11 567.22	.10	295
		3, 0, 3← 2, 1, 2	Ground			4		3	11 567.73	.10	295
		3, 0, 3← 2, 1, 2	Ground			3		2	11 569.21	.10	295
		3, 1, 2← 3, 1, 3	Ground			2		2	10 672.20	.10	295
		3, 1, 2← 3, 1, 3	Ground			4		4	10 672.88	.10	295
		3, 1, 2← 3, 1, 3	Ground			3		3	10 675.03	.10	295
		4, 0, 4← 3, 1, 3	Ground			5		4	35 782.59	.10	295
		4, 0, 4← 3, 1, 3	Ground			3		2	35 782.59	.10	295
		4, 0, 4← 3, 1, 3	Ground			4		3	35 783.93	.10	295
		4, 1, 3← 4, 1, 4	Ground			5		5	17 784.10	.10	295
		4, 1, 3← 4, 1, 4	Ground			3		3	17 784.10	.10	295
		4, 1, 3← 4, 1, 4	Ground			4		4	17 786.54	.10	295
		5, 1, 4← 5, 1, 5	Ground			6		6	26 664.83	.10	295
		5, 1, 4← 5, 1, 5	Ground			4		4	26 664.83	.10	295
		5, 1, 4← 5, 1, 5	Ground			5		5	26 667.27	.10	295
		5, 2, 4← 6, 1, 5	Ground	1		5		6	17 744.62	.10	295
		5, 2, 4← 6, 1, 5	Ground	1		4		5	17 745.95	.10	295
		5, 2, 4← 6, 1, 5	Ground	1		6		7	17 745.95	.10	295

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2N^{14}O^{16}H$	141	5, 2, 4← 6, 1, 5	Ground			5		6	20 332.08	.10	295
		5, 2, 4← 6, 1, 5	Ground			4		5	20 333.55	.10	295
		5, 2, 4← 6, 1, 5	Ground			6		7	20 333.55	.10	295
		7, 2, 5← 8, 1, 8	Ground			8		9	33 029.62	.10	295
		7, 2, 5← 8, 1, 8	Ground			6		7	33 029.62	.10	295
		7, 2, 5← 8, 1, 8	Ground			7		8	33 031.20	.10	295
		8, 1, 7← 7, 2, 6	Ground			9		8	35 878.00	.10	295
		8, 1, 7← 7, 2, 6	Ground			7		6	35 878.00	.10	295
		8, 1, 7← 7, 2, 6	Ground			8		7	35 879.33	.10	295
		8, 2, 6← 9, 1, 9	Ground	1		9		10	18 993.86	.10	295
		8, 2, 6← 9, 1, 9	Ground	1		7		8	18 993.86	.10	295
		8, 2, 6← 9, 1, 9	Ground	1		8		9	18 995.60	.10	295
		8, 2, 6← 9, 1, 9	Ground			9		10	22 992.67	.10	295
		8, 2, 6← 9, 1, 9	Ground			7		8	22 992.67	.10	295
		8, 2, 6← 9, 1, 9	Ground			8		9	22 994.40	.10	295
		9, 2, 7← 9, 2, 8	Ground			10		10	13 113.34	.10	295
		9, 2, 7← 9, 2, 8	Ground			8		8	13 113.34	.10	295
		9, 2, 7← 9, 2, 8	Ground			9		9	13 114.20	.10	295
		9, 2, 7←10, 1,10	Ground			10		11	15 265.32	.10	295
		9, 2, 7←10, 1,10	Ground			8		9	15 265.32	.10	295
		9, 2, 7←10, 1,10	Ground			9		10	15 267.31	.10	295
		10, 2, 8←10, 2, 9	Ground	1		11		11	18 770.96	.10	295
		10, 2, 8←10, 2, 9	Ground	1		9		9	18 770.96	.10	295
		10, 2, 8←10, 2, 9	Ground	1		10		10	18 771.93	.10	295
		10, 2, 8←10, 2, 9	Ground			11		11	19 226.21	.10	295
		10, 2, 8←10, 2, 9	Ground			9		9	19 226.21	.10	295
		10, 2, 8←10, 2, 9	Ground			10		10	19 227.17	.10	295
		10, 3, 8←11, 2, 9	Ground			10		11	22 021.47	.10	295
		10, 3, 8←11, 2, 9	Ground			9		10	22 022.37	.10	295
		10, 3, 8←11, 2, 9	Ground			11		12	22 022.37	.10	295
		11, 2, 9←11, 2,10	Ground			10		10	26 999.14	.10	295
		11, 2, 9←11, 2,10	Ground			12		12	26 999.14	.10	295
		11, 2, 9←11, 2,10	Ground			11		11	27 000.07	.10	295
		11, 3, 8←12, 2,11	Ground			10		11	31 633.09	.10	295
		11, 3, 8←12, 2,11	Ground			12		13	31 633.09	.10	295
		11, 3, 8←12, 2,11	Ground			11		12	31 633.42	.10	295
		12, 3, 9←13, 2,12	Ground			11		12	14 294.70	.10	295
		12, 3, 9←13, 2,12	Ground			13		14	14 294.70	.10	295
		12, 3, 9←13, 2,12	Ground			12		13	14 295.11	.10	295
		16, 3,13←16, 3,14	Ground			15		15	15 105.64	.10	295
		16, 3,13←16, 3,14	Ground			17		17	15 105.64	.10	295
		16, 3,13←16, 3,14	Ground			16		16	15 106.03	.10	295
		17, 3,14←17, 3,15	Ground			18		18	20 993.06	.10	295
		17, 3,14←17, 3,15	Ground			16		16	20 993.06	.10	295
		17, 3,14←17, 3,15	Ground			17		17	20 993.56	.10	295
$C^{12}H_2N^{14}O^{16}D$	142	1, 0, 1← 0, 0, 0				2		1	20 566.08	.10	295
		1, 0, 1← 0, 0, 0				1		1	20 566.97	.10	295
		1, 1, 1← 2, 0, 2	Ground	1		1		2	12 791.54	.10	295
		1, 1, 1← 2, 0, 2	Ground	1		2		3	12 793.90	.10	295
		1, 1, 1← 2, 0, 2	Ground			1		2	13 986.09	.10	295

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2N^{14}O^{16}D$	142	1, 1, 1← 2, 0, 2	Ground			2		3	13 988.28	.10	295
		1, 1, 1← 2, 0, 2	Ground			0		1	13 990.74	.10	295
		2, 0, 2← 1, 0, 1	Ground	1		2		1	41 095.53	.10	295
		2, 0, 2← 1, 0, 1	Ground	1		3		2	41 095.53	.10	295
		2, 0, 2← 1, 0, 1				1		1	41 096.43	.10	295
		2, 0, 2← 1, 0, 1				3		2	41 097.95	.10	295
		2, 0, 2← 1, 0, 1				2		1	41 097.95	.10	295
		2, 0, 2← 1, 0, 1				1		0	41 098.76	.10	295
		2, 0, 2← 1, 0, 1				2		2	41 098.76	.10	295
		2, 1, 1← 1, 1, 0				3		2	42 728.98	.10	295
		2, 1, 1← 1, 1, 0				1		0	42 728.98	.10	295
		2, 1, 2← 1, 1, 1				1		0	39 533.53	.10	295
		2, 1, 2← 1, 1, 1				3		2	39 535.25	.10	295
		2, 1, 2← 1, 1, 1				2		1	39 536.16	.10	295
		2, 1, 2← 1, 1, 1				1		1	39 536.88	.10	295
		2, 1, 2← 1, 1, 1	Ground	1		1		0	39 568.84	.10	295
		2, 1, 2← 1, 1, 1	Ground	1		3		2	39 570.50	.10	295
		2, 1, 2← 1, 1, 1	Ground	1		2		1	39 571.43	.10	295
		4, 0, 4← 3, 1, 3	Ground			5		4	30 677.65	.10	295
		4, 0, 4← 3, 1, 3	Ground			3		2	30 677.65	.10	295
		4, 0, 4← 3, 1, 3	Ground			4		3	30 679.05	.10	295
		5, 1, 4← 5, 1, 5	Ground	1		4		4	23 360.03	.10	295
		5, 1, 4← 5, 1, 5	Ground	1		6		6	23 360.03	.10	295
		5, 1, 4← 5, 1, 5	Ground	1		5		5	23 362.43	.10	295
		5, 1, 4← 5, 1, 5	Ground			6		6	23 938.78	.10	295
		5, 1, 4← 5, 1, 5	Ground			4		4	23 938.78	.10	295
		5, 1, 4← 5, 1, 5	Ground			5		5	23 941.21	.10	295
		5, 2, 4← 6, 1, 5	Ground	1		5		6	24 669.18	.10	295
		5, 2, 4← 6, 1, 5	Ground	1		4		5	24 670.63	.10	295
		5, 2, 4← 6, 1, 5	Ground	1		6		7	24 670.63	.10	295
		5, 2, 4← 6, 1, 5	Ground			5		6	27 911.82	.10	295
		5, 2, 4← 6, 1, 5	Ground			6		5	27 913.06	.10	295
		5, 2, 4← 6, 1, 5	Ground			6		7	27 913.06	.10	295
		8, 1, 7← 7, 2, 6	Ground			9		8	24 380.58	.10	295
		8, 1, 7← 7, 2, 6	Ground			7		6	24 380.58	.10	295
		8, 1, 7← 7, 2, 6	Ground			8		7	24 381.78	.10	295
		8, 2, 6← 9, 1, 9	Ground	1		7		8	22 238.36	.10	295
		8, 2, 6← 9, 1, 9	Ground	1		9		10	22 238.36	.10	295
		8, 2, 6← 9, 1, 9	Ground	1		8		9	22 240.09	.10	295
		8, 2, 6← 9, 1, 9	Ground			9		10	26 961.70	.10	295
		8, 2, 6← 9, 1, 9	Ground			7		8	26 961.70	.10	295
		8, 2, 6← 9, 1, 9	Ground			8		9	26 963.42	.10	295
		11, 2, 9←11, 2,10	Ground	1		10		10	21 834.41	.10	295
		11, 2, 9←11, 2,10	Ground	1		12		12	21 834.41	.10	295
		11, 2, 9←11, 2,10	Ground	1		11		11	21 835.32	.10	295
		11, 2, 9←11, 2,10	Ground			12		12	22 421.45	.10	295
		11, 2, 9←11, 2,10	Ground			10		10	22 421.45	.10	295
		11, 2, 9←11, 2,10	Ground			11		11	22 422.37	.10	295

CH_3NO $C_1(C_s,C_s)$ $HCONH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$HC^{12}O^{16}N^{14}H_2$	C_1	151	72 716.12 M	11 373.75 M	9 833.72 M				.0086
c-$HDN^{14}C^{12}HO^{16}$	C_1	152	61 345.91 M	11 009.91 M	9 334.09 M				.0029
t-$HDN^{14}C^{12}HO^{16}$	C_1	153	71 179.61 M	10 473.30 M	9 132.47 M				−.0154
$D_2N^{14}C^{12}HO^{16}$	C_1	154	59 715.99 M	10 193.58 M	8 710.35 M				−.0207
$H_2N^{14}C^{12}DO^{16}$	C_1	155	54 948.39 M	11 373.07 M	9 419.70 M				.0175
$H_2N^{15}C^{12}HO^{16}$	C_1	156	72 448.61 M	11 054.40 M	9 589.93 M				.0058
$H_2N^{15}C^{12}DO^{16}$	C_1	157	54 733.59 M	11 052.66 M	9 193.12 M				.0155
c-$HDN^{15}C^{12}HO^{16}$	C_1	158	61 275.15 M	10 721.79 M	9 124.91 M				.0011
t-$HDN^{15}C^{12}HO^{16}$	C_1	159	70 820.47 M	10 223.17 M	8 936.16 M				−.0163
$D_2N^{15}C^{12}HO^{16}$	C_1	161	59 594.17 M	9 964.80 M	8 540.45 M				−.0221

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
151	3.62 M	0.85 M						304 1			
152								229 1			
153								246 1			
154								170 1			

References:

ABC: 278 D_J: D_{JK}: κ: Δ: 278

μ: 177 eQq: V: I: ω: 278

eQq along the principal axes: $eQq_{aa} = 1.9$ MHz, $eQq_{bb} = 1.7$ MHz, and $eQq_{cc} = -3.6$ MHz. Barrier height (inversion-wagging mode) $= 1060 \pm 150$ cal/mol. Torsional frequency: for H_2 species is 600 ± 50 cm^{-1}; for D_2 species is 490 ± 40 cm^{-1}. Ref: 278, 142.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$HC^{12}O^{16}N^{14}H_2$	151	1, 0, 1← 0, 0, 0	1						21 190.7		278
		1, 0, 1← 0, 0, 0	Ground			0		1	21 206.56	.1	177
		1, 0, 1← 0, 0, 0	Ground			2		1	21 207.43	.1	177
		1, 0, 1← 0, 0, 0	Ground			1		1	21 207.96	.1	177
		1, 1, 1← 2, 0, 2	Ground			1		2	18 956.28	.1	177
		1, 1, 1← 2, 0, 2	Ground			0		1	18 956.28	.1	177
		1, 1, 1← 2, 0, 2	Ground			2		3	18 956.28	.1	177
		2, 0, 2← 1, 0, 1	Ground						42 386.07		278
		2, 1, 2← 1, 1, 1	Ground						40 874.91		278
		4, 0, 4← 3, 1, 3	Ground			4		3	26 924.05	.1	177
		4, 0, 4← 3, 1, 3	Ground			3		2	26 924.05	.1	177
		4, 0, 4← 3, 1, 3	Ground			5		4	26 924.05	.1	177
		4, 1, 3← 4, 1, 4	Ground			4		4	15 390.80	.1	177
		4, 1, 3← 4, 1, 4	Ground			5		5	15 392.71	.1	177
		4, 1, 3← 4, 1, 4	Ground			3		3	15 392.88	.1	177
		5, 1, 4← 5, 1, 5	Ground			5		5	23 080.06	.1	177
		5, 1, 4← 5, 1, 5	Ground			4		4	23 081.86	.1	177
		5, 1, 4← 5, 1, 5	Ground			6		6	23 082.26	.1	177
		6, 1, 5← 6, 1, 6	Ground			6		6	32 296.18	.1	177
		6, 1, 5← 6, 1, 6	Ground			7		7	32 298.19	.1	177
		6, 1, 5← 6, 1, 6	Ground			5		5	32 298.19	.1	177
		6, 2, 5← 7, 1, 6	Ground			5		6	16 960.96	.1	177
		6, 2, 5← 7, 1, 6	Ground			7		8	16 960.96	.1	177
		6, 2, 5← 7, 1, 6	Ground			6		7	16 960.96	.1	177
c-$HDN^{14}C^{12}HO^{16}$	152	1, 0, 1← 0, 0, 0	1						20 341.2		278
		1, 0, 1← 0, 0, 0	Ground						20 344.25	.1	177
		1, 1, 1← 2, 0, 2	Ground						9 689.15		278
		2, 0, 2← 1, 0, 1	Ground						40 647.52	.2	177
		2, 1, 1← 1, 1, 0	Ground						42 363.74		278
		2, 1, 2← 1, 1, 1	Ground						39 013.50	.2	177
		3, 0, 3← 2, 1, 2	Ground						12 166.33		278
		4, 0, 4← 3, 1, 3	Ground						34 639.00		278
		4, 2, 3← 5, 1, 4	Ground						39 492.18		278
		5, 1, 4← 5, 1, 5	Ground			5		5	25 113.15	.1	177
		5, 1, 4← 5, 1, 5	Ground			6		6	25 115.24	.1	177
		5, 1, 4← 5, 1, 5	Ground			4		4	25 115.24	.1	177
		7, 1, 6← 6, 2, 5	Ground						11 423.09		278
t-$HDN^{14}C^{12}HO^{16}$	153	1, 0, 1← 0, 0, 0	Ground						19 606.11	.1	177
		1, 0, 1← 0, 0, 0	1						19 621.6		278
		1, 1, 1← 2, 0, 2	Ground						21 516.74		278
		2, 0, 2← 1, 0, 1	Ground						39 190.40	.2	177
		2, 1, 1← 1, 1, 0	Ground						40 551.94	.2	177
		2, 1, 2← 1, 1, 1	Ground						37 870.72	.2	177
		4, 0, 4← 3, 1, 3	Ground						20 751.45		278
		5, 0, 5← 4, 1, 4	Ground						42 642.30		278
		5, 1, 4← 5, 1, 5	Ground			5		5	20 103.88	.1	177
		5, 1, 4← 5, 1, 5	Ground			4		4	20 105.84	.1	177
		5, 1, 4← 5, 1, 5	Ground			6		6	20 105.84	.1	177
		7, 1, 6← 6, 2, 5	Ground						28 596.20		278

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$D_2N^{14}C^{12}HO^{16}$	154	1, 0, 1← 0, 0, 0	Ground						18 904.01	.1	177
		1, 0, 1← 0, 0, 0	1						18 929.5		278
		1, 1, 1← 2, 0, 2	Ground						11 747.37		278
		2, 0, 2← 1, 0, 1	Ground						37 775.20	.2	177
		2, 1, 1← 1, 1, 0	Ground						39 290.66	.2	177
		2, 1, 2← 1, 1, 1	Ground						36 325.76	.2	177
		4, 0, 4← 3, 1, 3	Ground						29 328.44		278
		5, 1, 4← 5, 1, 5	Ground			5		5	22 229.78	.1	177
		5, 1, 4← 5, 1, 5	Ground			6		6	22 231.80	.1	177
		5, 1, 4← 5, 1, 5	Ground			4		4	22 231.80	.1	177
		6, 1, 5← 5, 2, 4	Ground						22 209.24		278
$H_2N^{14}C^{12}DO^{16}$	155	1, 0, 1← 0, 0, 0	Ground						20 792.77		278
		2, 0, 2← 1, 0, 1	Ground						41 521.85		278
		2, 1, 2← 1, 1, 1	Ground						39 632.17		278
		3, 0, 3← 2, 1, 2	Ground						20 435.77		278
		3, 2, 2← 4, 1, 3	Ground						40 883.81		278
		7, 1, 6← 6, 2, 5	Ground						37 765.17		278
$H_2N^{15}C^{12}HO^{16}$	156	1, 0, 1← 0, 0, 0	Ground						20 664.33		278
		1, 1, 1← 2, 0, 2	Ground						20 131.44		278
		2, 0, 2← 1, 0, 1	Ground						41 262.58		278
		2, 1, 2← 1, 1, 1	Ground						39 824.19		278
		4, 0, 4← 3, 1, 3	Ground						24 470.30		278
		7, 1, 6← 6, 2, 5	Ground						21 933.95		278
$H_2N^{15}C^{12}DO^{16}$	157	1, 0, 1← 0, 0, 0	Ground						20 245.78		278
		2, 0, 2← 1, 0, 1	Ground						40 433.42		278
		2, 1, 2← 1, 1, 1	Ground						38 632.02		278
		3, 0, 3← 2, 1, 2	Ground						18 625.75		278
		4, 0, 4← 3, 1, 3	Ground						41 117.81		278
		4, 2, 3← 5, 1, 4	Ground						19 029.94		278
		7, 1, 6← 6, 2, 5	Ground						32 595.74		278
c-$HDN^{15}C^{12}HO^{16}$	158	1, 0, 1← 0, 0, 0	Ground						19 846.70		278
		1, 1, 1← 2, 0, 2	Ground						10 897.20		278
		2, 0, 2← 1, 0, 1	Ground						39 655.90		278
		2, 1, 1← 1, 1, 0	Ground						41 290.30		278
		2, 1, 2← 1, 1, 1	Ground						38 096.52		278
		3, 0, 3← 2, 1, 2	Ground						10 397.83		278
		4, 0, 4← 3, 1, 3	Ground						32 289.71		278
		6, 1, 5← 5, 2, 4	Ground						18 679.65		278
t-$HDN^{15}C^{12}HO^{16}$	159	1, 0, 1← 0, 0, 0	Ground						19 159.33		278
		1, 1, 1← 2, 0, 2	Ground						22 298.92		278
		2, 0, 2← 1, 0, 1	Ground						38 298.26		278
		2, 1, 1← 1, 1, 0	Ground						39 605.82		278
		2, 1, 2← 1, 1, 1	Ground						37 031.65		278
		4, 0, 4← 3, 1, 3	Ground						18 964.62		278
		5, 0, 5← 4, 1, 4	Ground						40 332.08		278
$D_2N^{15}C^{12}HO^{16}$	161	1, 0, 1← 0, 0, 0	Ground						18 505.25		278
		1, 1, 1← 2, 0, 2	Ground						12 649.10		278
		2, 0, 2← 1, 0, 1	Ground						36 980.00		278
		2, 1, 1← 1, 1, 0	Ground						38 434.56		278
		2, 1, 2← 1, 1, 1	Ground						35 586.15		278
		4, 0, 4← 3, 1, 3	Ground						27 516.69		278
		6, 1, 5← 5, 2, 4	Ground						25 418.95		278

CH_3NO_2 $C_s(C_{3v},C_{2v})$ CH_3NO_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3N^{14}O_2^{16}$		171	13 277.5 M	10 542.7 M	5 876.7 M		.16		
$C^{12}D_3N^{14}O_2^{16}$		172	13 277.5 M	8 697.1 M	5 254.3 M		.12		

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_6	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
171	3.46 M				6.03	.03					
172					5.19	.03					

References:

ABC: 155 D_J: D_{JK}: 155 κ: Δ:

μ: 155 eQq: V: 155 I: ω:

Add. Refs.: 13, 19, 70, 99, 125, 265, 281

For species 171, $V_{12} < .05$ cal/mol. For species 172, $V_{12} < .05$ cal/mol. Ref: 155.

Nitromethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}O_2^{16}$	171	2, 0, ← 1, 0,	Ground						30 037.2	.2	155
		2, 0, ← 1, 0,	Ground						32 826.	2.	155
		2, 0, ← 1, 0,	Ground						32 859.5	.2	155
		2, 0, ← 1, 0,	Ground						32 959.2	.2	155
		2, 1, ← 1, 1,	Ground						31 677.3	.2	155
		2, 1, ← 1, 1,	Ground						32 034.1	.2	155
		2, 1, ← 1, 1,	Ground						32 189.7	.2	155
		2, 1, ← 1, 1,	Ground						32 660.	2.	155
		2, 1, ← 1, 1,	Ground						32 692.	2.	155
		2, 1, ← 1, 1,	Ground						32 921.	2.	155
		2, 1, ← 1, 1,	Ground						32 985.	2.	155
		2, 1, ← 1, 1,	Ground						33 476.5	.2	155
		2, 1, ← 1, 1,	Ground						33 643.5	.2	155
		2, 1, ← 1, 1,	Ground						33 988.5	.2	155
		3, 0, ← 2, 0,	Ground						41 534.9	.2	155

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}O_2^{16}$	171	Not Reported	Ground						16 199.43		132
		Not Reported	Ground						16 342.	5.	52
		Not Reported	Ground						16 407.48		132
		Not Reported	Ground						16 414.84		132
		Not Reported	Ground						16 419.50		132
		Not Reported	Ground						16 527.51		132
		Not Reported	Ground						16 561.51		132
		Not Reported	Ground						16 689.	5.	52
		Not Reported	Ground						16 721.81		132
		Not Reported	Ground						16 807.	5.	52
		Not Reported	Ground						16 823.	5.	52
		Not Reported	Ground						16 915.	5.	52
		Not Reported	Ground						16 948.	5.	52
		Not Reported	Ground						17 053.	5.	52
		Not Reported	Ground						17 228.	5.	52
		Not Reported	Ground						17 255.29		132
		Not Reported	Ground						17 346.40		132
		Not Reported	Ground						17 365.	5.	52
		Not Reported	Ground						17 462.	5.	52
		Not Reported	Ground						17 513.	5.	52
		Not Reported	Ground						17 530.	5.	52
		Not Reported	Ground						17 624.66		132
		Not Reported	Ground						17 645.77		132
		Not Reported	Ground						17 864.	5.	52
		Not Reported	Ground						17 904.86		132
		Not Reported	Ground						17 972.15		132
		Not Reported	Ground						18 068.	5.	52
		Not Reported	Ground						18 102.	5.	52
		Not Reported	Ground						18 112.	5.	52
		Not Reported	Ground						18 136.	5.	52
		Not Reported	Ground						18 172.	5.	52
		Not Reported	Ground						18 239.	5.	52
		Not Reported	Ground						18 256.	5.	52
		Not Reported	Ground						18 574.	5.	52
		Not Reported	Ground						18 609.	5.	52
		Not Reported	Ground						18 665.	5.	52
		Not Reported	Ground						18 794.95		132
		Not Reported	Ground						18 810.	5.	52
		Not Reported	Ground						18 817.69		132
		Not Reported	Ground						18 821.93		132
		Not Reported	Ground						18 938.	5.	52
		Not Reported	Ground						19 025.	5.	52
		Not Reported	Ground						19 055.	5.	52
		Not Reported	Ground						19 233.	5.	52
		Not Reported	Ground						19 370.	5.	52
		Not Reported	Ground						19 420.	5.	52
		Not Reported	Ground						19 468.86		132
		Not Reported	Ground						19 486.13		132
		Not Reported	Ground						19 509.18		132
		Not Reported	Ground						19 560.95		132
		Not Reported	Ground						19 576.	5.	52
		Not Reported	Ground						19 619.86		132
		Not Reported	Ground						19 719.	5.	52
		Not Reported	Ground						19 794.	5.	52
		Not Reported	Ground						19 828.	5.	52

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}O_2^{16}$	171	Not Reported	Ground						20 031.30		132
		Not Reported	Ground						20 084.41		132
		Not Reported	Ground						20 188.	5.	52
		Not Reported	Ground						20 260.	5.	52
		Not Reported	Ground						20 296.75		132
		Not Reported	Ground						20 385.		13
		Not Reported	Ground						20 405.	5.	52
		Not Reported	Ground						21 190.	5.	52
		Not Reported	Ground						21 500.	5.	52
		Not Reported	Ground						21 970.		19
		Not Reported	Ground						22 040.		70
		Not Reported	Ground						22 056.78		132
		Not Reported	Ground						22 068.	5.	52
		Not Reported	Ground						22 271.57		132
		Not Reported	Ground						22 332.	5.	52
		Not Reported	Ground						22 372.15		132
		Not Reported	Ground						22 393.96		132
		Not Reported	Ground						22 418.	5.	52
		Not Reported	Ground						22 465.		70
		Not Reported	Ground						22 478.	5.	52
		Not Reported	Ground						22 489.	5.	52
		Not Reported	Ground						22 528.	5.	52
		Not Reported	Ground						22 536.	5.	52
		Not Reported	Ground						22 580.		19
		Not Reported	Ground						22 620.		19
		Not Reported	Ground						22 628.	5.	52
		Not Reported	Ground						22 651.	5.	52
		Not Reported	Ground						22 701.	5.	52
		Not Reported	Ground						22 710.		70
		Not Reported	Ground						22 820.	5.	52
		Not Reported	Ground						22 830.		70
		Not Reported	Ground						23 004.	5.	52
		Not Reported	Ground						23 015.		70
		Not Reported	Ground						23 021.	5.	19
		Not Reported	Ground						23 250.		13
		Not Reported	Ground						23 260.		70
		Not Reported	Ground						23 293.91		132
		Not Reported	Ground						23 330.30		132
		Not Reported	Ground						23 458.88		132
		Not Reported	Ground						23 470.		70
		Not Reported	Ground						23 483.	5.	19
		Not Reported	Ground						23 499.	5.	52
		Not Reported	Ground						23 594.	5.	52
		Not Reported	Ground						23 652.02		132
		Not Reported	Ground						23 661.	5.	52
		Not Reported	Ground						23 668.03		132
		Not Reported	Ground						23 680.		70
		Not Reported	Ground						23 700.01		132
		Not Reported	Ground						23 706.	5.	19
		Not Reported	Ground						23 746.16		132

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}O_2^{16}$	171	Not Reported	Ground						23 754.	5.	52
		Not Reported	Ground						23 782.	5.	52
		Not Reported	Ground						23 798.	5.	52
		Not Reported	Ground						23 896.	5.	52
		Not Reported	Ground						23 939.	5.	52
		Not Reported	Ground						24 017.	5.	19
		Not Reported	Ground						24 047.		13
		Not Reported	Ground						24 140.	5.	52
		Not Reported	Ground						24 286.	5.	52
		Not Reported	Ground						24 320.		13
		Not Reported	Ground						24 338.	5.	52
		Not Reported	Ground						24 386.	5.	52
		Not Reported	Ground						24 420.	5.	52
		Not Reported	Ground						24 428.	5.	19
		Not Reported	Ground						24 437.80		132
		Not Reported	Ground						24 445.		70
		Not Reported	Ground						24 506.	5.	52
		Not Reported	Ground						24 592.85		132
		Not Reported	Ground						24 599.	5.	19
		Not Reported	Ground						24 605.		70
		Not Reported	Ground						24 658.	5.	52
		Not Reported	Ground						24 687.00		132
		Not Reported	Ground						24 879.62		132
		Not Reported	Ground						24 959.	5.	52
		Not Reported	Ground						25 224.	5.	52
		Not Reported	Ground						25 371.95		132
		Not Reported	Ground						25 394.28		132
		Not Reported	Ground						25 403.82		132
		Not Reported	Ground						25 412.	5.	19
		Not Reported	Ground						25 420.		70
		Not Reported	Ground						25 684.	5.	52
		Not Reported	Ground						25 701.	5.	52
		Not Reported	Ground						25 877.28		132
		Not Reported	Ground						25 912.55		132
		Not Reported	Ground						25 923.90		132
		Not Reported	Ground						25 942.44		132
		Not Reported	Ground						25 971.05		132
		Not Reported	Ground						26 024.73		132
		Not Reported	Ground						28 268.49		132
		Not Reported	Ground						29 572.23		132
		Not Reported	Ground						29 797.36		132
		Not Reported	Ground						30 526.20		132
		Not Reported	Ground						30 754.75		132
		Not Reported	Ground						30 768.28		132
		Not Reported	Ground						30 784.13		132
		Not Reported	Ground						30 795.32		132
		Not Reported	Ground						31 024.47		132
		Not Reported	Ground						31 052.99		132
		Not Reported	Ground						32 192.21		132
		Not Reported	Ground						32 446.09		132
		Not Reported	Ground						32 595.16		132
		Not Reported	Ground						32 827.63		132
		Not Reported	Ground						32 851.00		132
		Not Reported	Ground						32 858.99		132
		Not Reported	Ground						32 953.30		132

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}O_2^{16}$	171	Not Reported	Ground						32 970.81		132
		Not Reported	Ground						32 995.86		132
		Not Reported	Ground						33 292.34		132
		Not Reported	Ground						33 345.34		132
		Not Reported	Ground						33 376.80		132
		Not Reported	Ground						33 396.58		132
		Not Reported	Ground						33 477.35		132
		Not Reported	Ground						33 896.63		132
		Not Reported	Ground						33 904.84		132
		Not Reported	Ground						33 908.06		132
		Not Reported	Ground						33 929.63		132
		Not Reported	Ground						33 984.11		132
		Not Reported	Ground						33 995.68		132
		Not Reported	Ground						34 032.79		132
		Not Reported	Ground						34 040.42		132
		Not Reported	Ground						35 511.81		132
		Not Reported	Ground						35 521.62		132
		Not Reported	Ground						35 655.46		132
		Not Reported	Ground						36 815.0		132
		Not Reported	Ground						36 830.0		132
		Not Reported	Ground						36 941.21		132
		Not Reported	Ground						36 954.07		132
		Not Reported	Ground						36 984.23		132
		Not Reported	Ground						37 061.79		132
		Not Reported	Ground						37 210.6		132
		Not Reported	Ground						37 215.17		132
		Not Reported	Ground						37 254.66		132
		Not Reported	Ground						37 622.16		132
		Not Reported	Ground						37 659.84		132
		Not Reported	Ground						38 680.78		132
		Not Reported	Ground						39 531.29		132
		Not Reported	Ground						39 642.64		132
		Not Reported	Ground						39 804.42		132
		Not Reported	Ground						39 809.83		132
		Not Reported	Ground						39 917.60		132
		Not Reported	Ground						39 942.66		132
		Not Reported	Ground						40 035.48		132
		Not Reported	Ground						40 070.6		132
		Not Reported	Ground						40 106.6		132
		Not Reported	Ground						40 229.30		132
		Not Reported	Ground						40 285.16		132
		Not Reported	Ground						40 338.98		132
		Not Reported	Ground						40 386.20		132
		Not Reported	Ground						40 411.32		132
		Not Reported	Ground						40 582.20		132
		Not Reported	Ground						40 606.69		132
		Not Reported	Ground						40 682.11		132
		Not Reported	Ground						40 799.31		132
		Not Reported	Ground						40 898.49		132
		Not Reported	Ground						41 040.98		132

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3N^{14}O_2^{16}$	172	2, 0, ← 1, 0,	Ground						26 572.5	.2	155
		2, 0, ← 1, 0,	Ground						27 894.8	.2	155
		2, 0, ← 1, 0,	Ground						27 916.7	.2	155
		2, 0, ← 1, 0,	Ground						27 987.7	.2	155
		2, 1, ← 1, 1,	Ground						27 176.6	.2	155
		2, 1, ← 1, 1,	Ground						27 461.1	.2	155
		2, 1, ← 1, 1,	Ground						27 470.	2.0	155
		2, 1, ← 1, 1,	Ground						27 804.	2.0	155
		2, 1, ← 1, 1,	Ground						27 816.	2.0	155
		2, 1, ← 1, 1,	Ground						27 944.	2.0	155
		2, 1, ← 1, 1,	Ground						27 978.	2.0	155
		2, 1, ← 1, 1,	Ground						28 327.9	.2	155
		2, 1, ← 1, 1,	Ground						28 344.	2.0	155
		2, 1, ← 1, 1,	Ground						28 621.6	.2	155
		2, 3, ← 2, 1,	Ground						33 264.	1.0	155
		3, 0, ← 2, 0,	Ground						37 465.3	.2	155
		3, 0, ← 2, 0,	Ground						41 792.5	1.0	155
		3, 0, ← 2, 0,	Ground						41 827.5	1.0	155
		3, 0, ← 2, 0,	Ground						41 864.	1.0	155
		3, 0, ← 2, 0,	Ground						41 924.8	.2	155
		3, 0, ← 2, 0,	Ground						42 187.2	.2	155
		3, 1, ← 2, 1,	Ground						40 922.9	.2	155
		3, 1, ← 2, 1,	Ground						41 253.7	.2	155
		3, 1, ← 2, 1,	Ground						41 736.0	.2	155
		3, 1, ← 2, 1,	Ground						41 745.6	.2	155
		3, 1, ← 2, 1,	Ground						41 924.9	.2	155
		3, 1, ← 2, 1,	Ground						41 995.4	.2	155
		3, 1, ← 2, 1,	Ground						42 640.	2.0	155
		3, 1, ← 2, 1,	Ground						42 906.8	.2	155
		3, 1, ← 2, 1,	Ground						42 980.2	.2	155
		3, 2, ← 2, 2,	Ground						40 983.2	.2	155
		3, 2, ← 2, 2,	Ground						41 467.2	.2	155
		3, 2, ← 2, 2,	Ground						41 592.7	.2	155
		3, 2, ← 2, 2,	Ground						41 638.	2.0	155
		3, 2, ← 2, 2,	Ground						41 856.	1.0	155
		3, 2, ← 2, 2,	Ground						41 966.	2.0	155
		3, 2, ← 2, 2,	Ground						42 030.	2.0	155
		3, 2, ← 2, 2,	Ground						42 391.4	.2	155

CH_3NO_3 $C_s(C_{3v},C_{2v},C_{2v})$ CH_3ONO_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3O^{16}N^{14}O_2^{16}$	C_s	181	11 795.06 M	4 707.52 M	3 438.29 M			−.6962	.019
$C^{12}D_3O^{16}N^{14}O_2^{16}$	C_s	182	11 030.54 M	4 124.97 M	3 121.87 M				
s-$C^{12}H_2DO^{16}N^{14}O_2^{16}$	C_s	183	11 657.1 M	4 427.23 M	3 276.39 M				
a-$C^{12}H_2DO^{16}N^{14}O_2^{16}$	C_1	184	11 485.2 M	4 524.25 M	3 347.67 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
181	3.08 M	0.25 M	0. X		2321			340 1			

1. Statistical entropy for this molecule is reported as 72.15 cal/deg. Third law entropy is reported as 75.89 cal/deg. The discrepancy is not understood.

References:

ABC: 317 D_J: D_{JK}: κ: 317 Δ: 317

μ: 317 eQq: V: 317. I: ω: 373

V_2 $(NO_2)=9100\pm2600$ cal/mol. Torsional frequency $(NO_2)=130\pm20$ cm^{-1}. $V_3(CH_3)=2321$ cal/mol. Torsional frequency $(CH_3)=188.5$ cm^{-1}. Constants for excited (NO_2) torsional states: for v=1, $I_a=43.115$ amu Å², $I_b=107.463$ amu Å², and $I_c=146.850$ amu Å²; for v=2, $I_a=43.356$ amu Å², $I_b=107.545$ amu Å², and $I_c=146.683$ amu Å². Ref: 317.

Methyl Nitrate

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3O^{16}N^{14}O_2^{16}$	181	1, 0, 1← 0, 0, 0	Ground							8 145.90	.2	317
		2, 0, 2← 1, 0, 1	Ground	E	2					16 048.11	.1	317
		2, 0, 2← 1, 0, 1	Ground	A	2					16 058.80	.1	317
		2, 0, 2← 1, 0, 1	Ground							16 135.85	.1	317
		2, 0, 2← 1, 0, 1	Ground		1					16 138.27	.1	317
		2, 0, 2← 1, 0, 1	Ground		2					16 139.49	.1	317
		2, 1, 1← 1, 1, 0	Ground	A	2					17 468.25	.1	317
		2, 1, 1← 1, 1, 0	Ground		2					17 548.41	.1	317
		2, 1, 1← 1, 1, 0	Ground		1					17 555.17	.1	317
		2, 1, 1← 1, 1, 0	Ground							17 560.84	.1	317
		2, 1, 2← 1, 1, 1	Ground							15 022.38	.1	317
		2, 1, 2← 1, 1, 1	Ground		1					15 031.69	.1	317
		2, 1, 2← 1, 1, 1	Ground		2					15 039.95	.1	317
		3, 0, 3← 2, 0, 2	Ground	E	2					23 706.45	.1	317
		3, 0, 3← 2, 0, 2	Ground	A	2					23 721.64	.1	317
		3, 0, 3← 2, 0, 2	Ground							23 829.45	.1	317
		3, 0, 3← 2, 0, 2	Ground		1					23 834.15	.1	317
		3, 0, 3← 2, 0, 2	Ground		2					23 837.43	.1	317
		3, 0, 3← 2, 0, 2	Ground		3					23 839.80	.1	317
		3, 1, 2← 2, 1, 1	Ground	E	2					26 041.92	.1	317

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3O^{16}N^{14}O_2^{16}$	181	3, 1, 2← 2, 1, 1	Ground	A	2					26 101.23	.1	317
		3, 1, 2← 2, 1, 1	Ground		4					26 197.05	.1	317
		3, 1, 2← 2, 1, 1	Ground		3					26 208.24	.1	317
		3, 1, 2← 2, 1, 1	Ground		2					26 219.05	.1	317
		3, 1, 2← 2, 1, 1	Ground		1					26 228.62	.1	317
		3, 1, 2← 2, 1, 1	Ground							26 237.30	.1	317
		3, 1, 3← 2, 1, 2	Ground	A	2					22 340.04	.1	317
		3, 1, 3← 2, 1, 2	Ground	E	2					22 365.79	.1	317
		3, 1, 3← 2, 1, 2	Ground							22 441.53	.1	317
		3, 2, 1← 2, 2, 0	Ground							25 044.80	.1	317
		3, 2, 2← 3, 0, 3	Ground							31 652.05	.1	317
		4, 0, 4← 3, 0, 3	Ground	E	2					30 997.1	.5	317
		4, 0, 4← 3, 0, 3	Ground	A	2					31 016.82	.1	317
		4, 0, 4← 3, 0, 3	Ground							31 149.42	.1	317
		4, 0, 4← 3, 0, 3	Ground		1					31 157.90	.1	317
		4, 0, 4← 3, 0, 3	Ground		2					31 165.00	.1	317
		4, 1, 3← 3, 1, 2	Ground	E	2					34 546.63	.1	317
		4, 1, 3← 3, 1, 2	Ground							34 771.44	.1	317
		4, 1, 4← 3, 1, 3	Ground	A	2					29 633.65	.1	317
		4, 1, 4← 3, 1, 3	Ground	E	2					29 637.	2.	317
		4, 1, 4← 3, 1, 3	Ground							29 765.97	.1	317
		4, 1, 4← 3, 1, 3	Ground		1					29 785.75	.1	317
		4, 2, 2← 3, 2, 1	Ground							33 893.	5.	317
		4, 2, 3← 3, 2, 2	Ground							32 461.38	.1	317
		4, 3, 1← 3, 3, 0	Ground							32 932.75	.1	317
		4, 1, 4← 4, 1, 3	Ground							12 609.40	.1	317
		4, 2, 3← 4, 0, 4	Ground							32 964.20	.1	317
		6, 2, 5← 6, 2, 4	Ground							8 688.00	.1	317
		9, 3, 7← 9, 3, 6	Ground							8 300.64	.1	317
$C^{12}D_3O^{16}N^{14}O_2^{16}$	182	2, 0, 2← 1, 0, 1	Ground							14 396.45	.1	317
		2, 1, 1← 1, 1, 0	Ground							15 501.59	.1	317
		3, 0, 3← 2, 0, 2	Ground							21 347.74	.1	317
		3, 1, 2← 2, 1, 1	Ground							23 185.23	.1	317
		3, 1, 3← 2, 1, 2	Ground							20 181.61	.1	317
s-$C^{12}H_2DO^{16}N^{14}O_2^{16}$	183	2, 0, 2← 1, 0, 1	Ground							15 280.53	.1	317
		2, 1, 1← 1, 1, 0	Ground							16 558.08	.1	317
		2, 1, 2← 1, 1, 1	Ground							14 256.37	.1	317
		4, 0, 4← 3, 0, 3	Ground							29 629.85	.1	317
a-$C^{12}H_2DO^{16}N^{14}O_2^{16}$	184	2, 0, 2← 1, 0, 1	Ground							15 606.90	.1	317
		2, 1, 1← 1, 1, 0	Ground							16 920.42	.1	317
		2, 1, 2← 1, 1, 1	Ground							14 567.27	.1	317
		3, 0, 3← 2, 0, 2	Ground							23 080.34	.1	317
		4, 0, 4← 3, 0, 3	Ground							30 217.30	.1	317

CH_4F_2Si $C_s(C_{3v},C_s)$ CH_3SiHF_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Si^{28}HF_2^{19}$-A	C_s	191	6 847.25 M	6 120.40 M	3 755.61 M				
$C^{12}H_3Si^{28}HF_2^{19}$-E	C_s	192	6 846.33 M	6 120.40 M	3 755.61 M				
$C^{12}H_3Si^{29}HF_2^{19}$	C_s	193	6 835.39 M	6 111.15 M	3 755.66 M				
$C^{12}H_3Si^{30}HF_2^{19}$	C_s	194	6 825.69 M	6 102.07 M	3 755.64 M				
$C^{13}H_3Si^{28}HF_2^{19}$-A	C_s	195	6 843.27 M	5 897.90 M	3 671.67 M				
$C^{13}H_3Si^{28}HF_2^{19}$-E	C_s	196	6 842.33 M	5 897.90 M	3 671.67 M				
$C^{12}H_3Si^{28}DF_2^{19}$-A	C_s	197	6 556.15 M	5 885.07 M	3 754.35 M				
$C^{12}H_3Si^{28}DF_2^{19}$-E	C_s	198	6 555.19 M	5 885.07 M	3 754.35 M				
$C^{12}D_3Si^{28}DF_2^{19}$	C_s	199	6 258.43 M	5 002.52 M	3 377.71 M				
$C^{12}D_3Si^{29}DF_2^{19}$	C_s	201	6 276.31 M	4 996.50 M	3 377.63 M				
s-$C^{12}H_2DSi^{28}HF_2^{19}$	C_s	203	6 [illegible]4.16 M	5 774.09 M	3 663.21 M				
a-$C^{12}H_2DSi^{28}HF_2^{19}$	C_1	204	6 796.64 M	5 737.71 M	3 596.89 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
191	2.01 M	0. X	0.62 M		1255	30					

References:

ABC: 23, 29, 234, 290 D_J: D_{JK}: κ: Δ:

μ: 234 eQq: V: 234 I: ω:

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Si^{28}HF_2^{19}$-A	191	2, 0, 2← 1, 0, 1	Ground	A	0					17 970.57		234
		2, 1, 1← 1, 0, 1	Ground	A	0					25 208.47		234
		2, 1, 1← 1, 1, 0	Ground	A	0					22 116.80		234
		2, 1, 2← 1, 1, 1	Ground	A	0					17 387.22		234
		2, 2, 0← 1, 1, 0	Ground	A	0					26 078.78		234
		2, 2, 1← 1, 1, 1	Ground	A	0					26 662.15		234
		3, 0, 3← 2, 0, 2	Ground	A	0					25 304.74		234
		3, 1, 2← 2, 1, 1	Ground	A	0					31 124.90		234
		3, 1, 3← 2, 1, 2	Ground	A	0					25 179.49		234
		3, 2, 1← 2, 2, 0	Ground	A	0					33 951.02		234
		3, 2, 2← 2, 2, 1	Ground	A	0					29 627.82		234
		6, 1, 6← 6, 1, 5	Ground	A	0					29 667.8		154
		7, 2, 6← 7, 2, 5	Ground	A	0					29 552.40		154
		7, 3, 5← 7, 3, 4	Ground	A	0					23 745.10		154
		8, 3, 6← 8, 3, 5	Ground							29 360.07		154
		8, 4, 5← 8, 4, 4	Ground		0					23 128.45		154
		9, 4, 6← 9, 4, 5	Ground							29 052.30		154
		9, 5, 5← 9, 5, 4	Ground	A	0					22 051.38		154
		10, 5, 6←10, 5, 5	Ground							28 540.65		154
		10, 6, 5←10, 6, 4	Ground	A	0					20 369.85		154
		11, 6, 6←11, 6, 5	Ground	A	0					27 688.80		154
		11, 7, 5←11, 7, 4	Ground	A	0					18 063.86		154
		12, 7, 6←12, 7, 5	Ground	A	0					26 319.80		154
		Not Reported	Ground							17 416.0		154
		Not Reported	Ground							17 462.4		154
		Not Reported	Ground							17 647.2		154
		Not Reported	Ground							17 717.1		154
		Not Reported	Ground							17 719.3		154
		Not Reported	Ground							17 817.1		154
		Not Reported	Ground							18 147.8		154
		Not Reported	Ground							18 150.2		154
		Not Reported	Ground							18 292.3		154
		Not Reported	Ground							18 403.1		154
		Not Reported	Ground							18 761.6		154
		Not Reported	Ground							24 060.7		154
		Not Reported	Ground							24 064.1		154
		Not Reported	Ground							24 086.7		154
		Not Reported	Ground							24 092.5		154
		Not Reported	Ground							24 236.3		154
		Not Reported	Ground							24 238.2		154
		Not Reported	Ground							24 267.4		154
		Not Reported	Ground							24 282.8		154
		Not Reported	Ground							24 293.7		154
		Not Reported	Ground							25 069.6		154
		Not Reported	Ground							25 145.6		154
		Not Reported	Ground							25 173.4		154
		Not Reported	Ground							25 221.9		154
		Not Reported	Ground							25 383.5		154
		Not Reported	Ground							25 598.7		154
		Not Reported	Ground							25 649.2		154

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_I'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Si^{28}HF_2^{19}$-A	191	Not Reported	Ground							27 688.9		154
		Not Reported	Ground							28 871.5		154
		Not Reported	Ground							28 873.4		154
		Not Reported	Ground							28 910.4		154
		Not Reported	Ground							28 914.3		154
		Not Reported	Ground							29 018.2		154
		Not Reported	Ground							29 088.5		154
		Not Reported	Ground							29 204.6		154
		Not Reported	Ground							29 219.2		154
		Not Reported	Ground							29 336.4		154
		Not Reported	Ground							29 343.8		154
		Not Reported	Ground							29 625.6		154
$C^{12}H_3Si^{28}HF_2^{19}$-E	192	2, 0, 2← 1, 0, 1	Ground	E	0					17 970.08		234
		2, 1, 1← 1, 0, 1	Ground	E	0					25 207.67		234
		2, 1, 1← 1, 1, 0	Ground	E	0					22 116.80		234
		2, 1, 2← 1, 1, 1	Ground	E	0					17 387.22		234
		2, 2, 0← 1, 1, 0	Ground	E	0					26 076.68		234
		2, 2, 1← 1, 1, 1	Ground	E	0					26 659.23		234
		3, 0, 3← 2, 0, 2	Ground	E	0					25 302.51		234
		3, 1, 2← 2, 1, 1	Ground	E	0					31 123.75		234
		3, 1, 3← 2, 1, 2	Ground	E	0					25 180.66		234
		3, 2, 1← 2, 2, 0	Ground	E	0					33 951.02		234
		3, 2, 2← 2, 2, 1	Ground	E	0					29 627.82		234
		6, 1, 6← 6, 1, 5	Ground	E	0					29 662.8		154
		7, 2, 6← 7, 2, 5	Ground	E	0					29 549.49		154
		7, 3, 5← 7, 3, 4	Ground	E	0					23 744.20		154
		9, 5, 5← 9, 5, 4	Ground	E	0					22 054.51		154
		10, 6, 5←10, 6, 4	Ground	E	0					20 377.40		154
		11, 6, 6←11, 6, 5	Ground	E	0					27 690.15		154
		11, 7, 5←11, 7, 4	Ground	E	0					18 074.90		154
		12, 7, 6←12, 7, 5	Ground	E	0					26 326.02		154
$C^{12}H_3Si^{29}HF_2^{19}$	193	2, 0, 2← 1, 0, 1	Ground		0					17 959.50		234
		2, 1, 1← 1, 1, 0	Ground	E	0					22 089.10		234
		2, 1, 1← 1, 1, 0	Ground	A	0					22 089.10		234
		2, 1, 2← 1, 1, 1	Ground	A	0					17 378.12		234
		2, 1, 2← 1, 1, 1	Ground	E	0					17 378.12		234
		3, 0, 3← 2, 0, 2	Ground	E	0					25 292.55		234
		3, 0, 3← 2, 0, 2	Ground	A	0					25 294.58		234
		3, 1, 2← 2, 1, 1	Ground		0					31 091.11		234
		3, 1, 3← 2, 1, 2	Ground	A	0					25 170.35		234
		3, 1, 3← 2, 1, 2	Ground	E	0					25 171.55		234
		3, 2, 2← 2, 2, 1	Ground	A	0					29 600.40		234
		3, 2, 2← 2, 2, 1	Ground	A	0					29 600.40		234
$C^{12}H_3Si^{30}HF_2^{19}$	194	2, 0, 2← 1, 0, 1	Ground		0					17 949.49		234
		2, 1, 1← 1, 1, 0	Ground	A	0					22 061.84		234
		2, 1, 1← 1, 1, 0	Ground	E	0					22 061.84		234
		3, 0, 3← 2, 0, 2	Ground	E	0					25 282.51		234
		3, 0, 3← 2, 0, 2	Ground	A	0					25 284.83		234
		3, 1, 3← 2, 1, 2	Ground		0					25 160.94		234

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Si^{30}HF_2^{19}$	194	3, 2, 2← 2, 2, 1	Ground	A	0					29 573.50		234
		3, 2, 2← 2, 2, 1	Ground	E	0					29 573.50		234
$C^{13}H_3Si^{28}HF_2^{19}$-A	195	2, 0, 2← 1, 0, 1	Ground	A	0					17 615.39		234
		2, 1, 1← 1, 1, 0	Ground	A	0					21 365.37		234
		2, 1, 2← 1, 1, 1	Ground	A	0					16 912.91		234
		3, 0, 3← 2, 0, 2	Ground	A	0					24 794.63		234
		3, 1, 2← 2, 1, 1	Ground	A	0					30 420.24		234
		3, 1, 3← 2, 1, 2	Ground		0					24 592.56		234
		3, 2, 1← 2, 2, 0	Ground	A	0					32 622.61		234
		3, 2, 2← 2, 2, 1	Ground	A	0					28 708.60		234
$C^{13}H_3Si^{28}HF_2^{19}$-E	196	2, 0, 2← 1, 0, 1	Ground	E	0					17 614.88		234
		2, 1, 1← 1, 1, 0	Ground	E	0					21 365.37		234
		2, 1, 2← 1, 1, 1	Ground	E	0					16 912.91		234
		3, 0, 3← 2, 0, 2	Ground	E	0					24 793.40		234
		3, 1, 2← 2, 1, 1	Ground	E	0					30 419.40		234
		3, 2, 1← 2, 2, 0	Ground	E	0					32 622.61		234
		3, 2, 2← 2, 2, 1	Ground	E	0					28 708.60		234
$C^{12}H_3Si^{28}DF_2^{19}$-A	197	2, 0, 2← 1, 0, 1	Ground	A	0					17 684.10		234
		2, 1, 1← 1, 1, 0	Ground	A	0					21 409.56		234
		2, 1, 2← 1, 1, 1	Ground	A	0					17 148.13		234
		3, 0, 3← 2, 0, 2	Ground	A	0					25 032.63		234
		3, 1, 2← 2, 1, 1	Ground	A	0					30 288.46		234
		3, 1, 3← 2, 1, 2	Ground	A	0					24 914.95		234
		3, 2, 1← 2, 2, 0	Ground	A	0					32 803.71		234
		3, 2, 2← 2, 2, 1	Ground	A	0					28 917.93		234
		7, 2, 6← 7, 2, 5	Ground	A	0					26 996.8		154
		11, 6, 6←11, 6, 5	Ground	A	0					24 904.4		154
		12, 7, 6←12, 7, 5	Ground	A	0					23 583.7		154
		Not Reported	Ground	A	0					16 952.9		154
		Not Reported	Ground	A	0					21 661.4		154
		Not Reported	Ground	A	0					21 763.5		154
		Not Reported	Ground	A	0					21 766.5		154
		Not Reported	Ground	A	0					27 262.5		154
		Not Reported	Ground	A	0					27 272.0		154
		Not Reported	Ground	A	0					28 849.1		154
		Not Reported	Ground	A	0					28 853.3		154
		Not Reported	Ground	A	0					29 911.8		154
$C^{12}H_3Si^{28}DF_2^{19}$-E	198	2, 0, 2← 1, 0, 1	Ground	E	0					17 683.49		234
		2, 1, 1← 1, 1, 0	Ground	E	0					21 409.56		234
		2, 1, 2← 1, 1, 1	Ground	E	0					17 148.13		234
		3, 0, 3← 2, 0, 2	Ground	E	0					25 030.55		234
		3, 1, 2← 2, 1, 1	Ground	E	0					30 287.49		234
		3, 1, 3← 2, 1, 2	Ground	E	0					24 916.13		234
		3, 2, 1← 2, 2, 0	Ground	E	0					32 803.71		234
		3, 2, 2← 2, 2, 1	Ground	E	0					28 917.93		234
		7, 2, 6← 7, 2, 5	Ground	E	0					26 993.5		154
		11, 6, 6←11, 6, 5	Ground	E	0					24 906.3		154
		12, 7, 6←12, 7, 5	Ground	E	0					23 589.7		154

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3Si^{28}DF_2^{19}$	199	2, 0, 2← 1, 0, 1	Ground						15 903.16	.1	290
		2, 1, 1← 1, 0, 1	Ground						21 292.84	.1	290
		2, 1, 1← 1, 1, 0	Ground						18 385.27	.1	290
		2, 1, 2← 1, 1, 1	Ground						15 135.65	.1	290 [1]
		2, 2, 0← 1, 1, 0	Ground						23 091.31	.1	290
		2, 2, 1← 1, 1, 1	Ground						23 858.82	.1	290
		3, 0, 3← 2, 0, 2	Ground						22 627.94	.1	290
		3, 1, 2← 2, 1, 1	Ground						26 796.36	.1	290
		3, 1, 3← 2, 1, 2	Ground						22 255.23	.1	290 [1]
		3, 2, 1← 2, 2, 0	Ground						27 653.13	.1	290
		3, 2, 2← 2, 2, 1	Ground						25 140.47	.1	290
$C^{12}D_3Si^{29}DF_2^{19}$	201	2, 0, 2← 1, 0, 1	Ground						15 894.60	2.	290
		2, 1, 1← 1, 1, 0	Ground						18 367.14	2.	290
		3, 0, 3← 2, 0, 2	Ground						22 620.04	2.	290
		3, 1, 3← 2, 1, 2	Ground						22 247.70	2.	290
		3, 2, 2← 2, 2, 1	Ground						25 122.39	2.	290
$C^{12}D_3Si^{30}DF_2^{19}$	202	2, 0, 2← 1, 0, 1	Ground						15 885.81	2.	290
		2, 1, 1← 1, 1, 0	Ground						18 349.40	2.	290
		3, 1, 3← 2, 1, 2	Ground						22 240.68	2.	290
		3, 2, 2← 2, 2, 1	Ground						25 103.39	2.	290
s-$C^{12}H_2DSi^{28}HF_2^{19}$	203	1, 0, 1← 0, 0, 0	Ground						9 437.10	2.	290
		2, 0, 2← 1, 0, 1	Ground						17 447.21	2.	290
		2, 1, 1← 1, 1, 0	Ground						20 985.49	2.	290
		2, 1, 2← 1, 1, 1	Ground						16 763.72	2.	290
		3, 0, 3← 2, 0, 2	Ground						24 620.48	2.	290
		3, 1, 2← 2, 1, 1	Ground						29 966.89	2.	290
		3, 1, 3← 2, 1, 2	Ground						24 417.34	2.	290
		3, 2, 1← 2, 2, 0	Ground						32 002.61	2.	290
		3, 2, 2← 2, 2, 1	Ground						28 311.60	2.	290
		4, 1, 4← 3, 1, 3	Ground						31 824.00	2.	290
a-$C^{12}H_2DSi^{28}HF_2^{19}$	204	1, 0, 1← 0, 0, 0	Ground						9 334.73	2.	290
		2, 0, 2← 1, 0, 1	Ground						17 281.36	2.	290
		2, 1, 1← 1, 1, 0	Ground						20 810.02	2.	290
		2, 1, 2← 1, 1, 1	Ground						16 528.39	2.	290
		3, 0, 3← 2, 0, 2	Ground						24 325.20	2.	290
		3, 0, 3← 2, 0, 2	Ground						24 328.18	2.	290
		3, 1, 2← 2, 1, 1	Ground						29 787.24	2.	290
		3, 1, 2← 2, 1, 1	Ground						29 789.34	2.	290
		3, 1, 3← 2, 1, 2	Ground						24 078.27	2.	290
		3, 1, 3← 2, 1, 2	Ground						24 083.22	2.	290
		3, 2, 1← 2, 2, 0	Ground						31 678.18	2.	290
		3, 2, 2← 2, 2, 1	Ground						28 004.28	2.	290
		4, 1, 4← 3, 1, 3	Ground						31 370.12	2.	290

1. Reassignments of two lines which the authors refer to as $2_{11}\leftarrow 1_{11}$ and $3_{13}\leftarrow 2_{11}$ have been made, since these assignments are forbidden. These lines are taken to be $2_{12}\leftarrow 1_{11}$ and $3_{12}\leftarrow 2_{12}$ respectively.

CH_4O $C_s(C_{3v},C_s)$ CH_3OH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3O^{16}H$	C_s	211	127 602.57 M	24 629.2 M	23 761.0 M		0.3681	−.98	
$C^{12}H_3O^{16}D$	C_s	212	109 536.86 M	23 395.3 M	21 968.5 M				
$C^{13}H_3O^{16}H$	C_s	213	127 600.63 M	24 018.3 M	23 191.9 M				
$C^{12}D_3O^{16}H$	C_s	214	70 511.82 M	19 822.8 M	19 256.0 M				
$C^{13}H_3O^{16}D$	C_s	215	109 534.00 M	22 794.7 M	21 438.0 M				
$C^{12}D_3O^{16}D$	C_s	216	64 627.78 M	18 868.0 M	17 928.8 M				
$C^{12}H_3O^{18}H$	C_s	217	127 333.42 M	23 590.4 M	22 784.1 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
211	0. X	1.440 M	0.885 M		1070						
212					371	5					
213	0. X	1.439 M	0.886 M								
217	0. X	1.437 M	0.890 M								

References:

ABC: 122 D_J: D_{JK}: 352 κ: 148 Δ:

μ: 54 eQq: V: 148, 344 I: ω:

Add. Refs.: 5, 6, 12, 14, 15, 22, 24, 25, 27, 35, 39, 51, 52, 54, 60, 72, 105, 120, 133, 169, 192, 208, 238, 240, 310, 351, 386

Torsional frequency = 270 cm^{-1}. Ref: 192.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_i'	F'	F_i	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3O^{16}H$	211	1, 0, 1← 0, 0, 0	Ground	A	2					48 178.0	1.	121
		1, 0, 1← 0, 0, 0	Ground	E	2					48 192.12	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	1					48 247.89	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	1					48 257.49	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	0					48 372.60	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	0					48 377.09	.5	121
		1, 0, 1← 0, 0, 0								49 867.2		396
		2, 2, ← 2, 1,	Ground	E(−)	0					24 934.38	.1	37
		2, 1, ← 3, 0,	Ground	E(−)	0					19 967.		72
		3, 1, ← 2, 0,	Ground	E(+)	0					12 178.6	.1	310
		3, 2, ← 3, 1,	Ground	E(−)	0					24 928.70	.1	37
		4, 0, ← 3, 1,	Ground	E(−)	0					28 316.03	.1	37
		4, 1, ← 3, 0,	Ground	E(+)	0					36 169.24	.1	37
		4, 2, ← 4, 1,	Ground	E(−)	0					24 933.47	.1	37
		4, 3, ← 5, 2,	Ground		0					10 002.		133
		5, 2, 3← 4, 3, 2	Ground							9 978.6	.1	280
		5, 2, 4← 4, 3, 1	Ground							10 058.3	.1	280
		5, 1, ← 5, 1,	Ground							12 511.0	.1	310
		5, 2, ← 5, 1,	Ground	E(−)	0					24 959.08	.1	37
		6, 2, ← 5, 3,	Ground	A	0					38 293.5	.1	37
		6, 2, ← 5, 3,	Ground	A	0					38 452.69	.1	37
		6, 2, ← 6, 1,	Ground	E(−)	0					25 018.14	.1	37
		7, 2, ← 7, 1,	Ground	E(−)	0					25 124.88	.1	37
		8, 2, ← 7, 1,	Ground	E(+)	0					37 703.72	.1	37
		8, 2, ← 8, 1,	Ground	E(−)	0					25 294.41	.1	37
		9, 1, ← 8, 2,	Ground	E(+)	0					9 936.2	.1	310
		9, 2, ← 9, 1,	Ground	E(−)	0					25 541.43	.1	37
		10, 2, ←10, 1,	Ground	E(−)	0					25 878.18	.1	37
		11, 2, ←11, 1,	Ground	E(−)	0					26 313.11	.1	37
		12, 2, ←12, 1,	Ground	E(−)	0					26 847.27	.1	37
		13, 2, ←13, 1,	Ground	E(−)	0					27 472.54	.1	37
		14, 2, ←14, 1,	Ground	E(−)	0					28 169.31	.1	37
		15, 2, ←15, 1,	Ground	E(−)	0					28 905.70	.1	37
		16, 2, ←16, 1,	Ground	E(−)	0					29 636.91	.1	37
		17, 2, ←17, 1,	Ground	E(−)	0					30 308.00	.1	37
		18, 2, ←18, 1,	Ground	E(−)	0					30 858.40	.1	37
		19, 2, ←19, 1,	Ground	E(−)	0					31 226.70	.1	37
		20, 2, ←20, 1,	Ground	E(−)	0					31 358.31	.1	37
		21, 2, ←21, 1,	Ground	E(−)	0					31 209.75	.1	37
		22, 2, ←22, 1,	Ground	E(−)	0					30 752.26	.1	37
		23, 2, ←23, 1,	Ground	E(−)	0					29 973.06	.1	37
		24, 2, ←24, 1,	Ground	E(−)	0					28 874.45	.1	37
		25, 2, ←25, 1,	Ground	E(−)	0					27 470.99	.1	37
		26, 2, ←26, 1,	Ground	E(−)	0					25 787.12	.1	37
		27, 2, ←27, 1,	Ground	E(−)	0					23 854.25	.1	37
		28, 2, ←28, 1,	Ground	E(−)	0					21 708.68	.1	37
		29, 2, ←29, 1,	Ground	E(−)	0					19 390.18	.1	37
		30, 2, ←30, 1,	Ground	E(−)	0					16 941.6	.1	37
		31, 2, ←31, 1,	Ground	E(−)	0					14 407.8	.1	310
		32, 2, ←32, 1,	Ground	E(−)	0					11 841.9	.1	310

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3O^{16}H$	211	33, 2, ←33, 1,	Ground	0					8 198.		133
		2, , ← 1, ,	Ground						8 380.		133
		8, , ← 7, ,	Ground						9 960.		133
		12, , ←11, ,	Ground						7 816.		133
		14, , ←13, ,	Ground						16 395.		133
		Not Reported	Ground						7 587.		133
		Not Reported	Ground						7 680.		133
		Not Reported	Ground						11 050.5	.1	310
		Not Reported	Ground						12 229.4	.1	310
		Not Reported	Ground						12 770.9	.1	310
		Not Reported	Ground						14 084.8	.1	310
		Not Reported	Ground						14 300.3	.1	310
		Not Reported	Ground						14 317.6	.1	310
		Not Reported	Ground						15 214.1	.1	310
		Not Reported	Ground						15 303.4	.1	310
		Not Reported	Ground						16 395.8	5.	52
		Not Reported	Ground						16 556.	5.	52
		Not Reported	Ground						17 507.	5.	52
		Not Reported	Ground						17 514.		133
		Not Reported	Ground						17 911.1	.1	37
		Not Reported	Ground						18 161.4	5.	52
		Not Reported	Ground						18 222.		133
		Not Reported	Ground						18 266.4	5.	52
		Not Reported	Ground						19 139.	5.	52
		Not Reported	Ground						19 162.		133
		Not Reported	Ground						19 252.		133
		Not Reported	Ground						20 171.07	.1	37
		Not Reported	Ground						20 346.83	.1	37
		Not Reported	Ground						20 898.	5.	12
		Not Reported	Ground						20 908.87	.1	37
		Not Reported	Ground						20 970.65	.1	37
		Not Reported	Ground						20 989.	5.	12
		Not Reported	Ground						21 244.2	.1	37
		Not Reported	Ground						21 550.31	.1	37
		Not Reported	Ground						22 095.	5.	12
		Not Reported	Ground						23 033.	5.	12
		Not Reported	Ground						23 121.20	.1	37
		Not Reported	Ground						23 347.53	.1	37
		Not Reported	Ground						23 415.	5.	12
		Not Reported	Ground						23 444.82	.1	37
		Not Reported	Ground						23 450.	5.	12
		Not Reported	Ground						23 457.	5.	19
		Not Reported	Ground						23 861.	5.	12
		Not Reported	Ground						24 040.	5.	12
		Not Reported	Ground						24 081.	5.	12
		Not Reported	Ground						24 317.	5.	12
		Not Reported	Ground						24 533.7	.1	37
		Not Reported	Ground						24 901.	5.	19
		Not Reported	Ground						24 913.	5.	19
		Not Reported							24 926.	5.	15

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3O^{16}H$	211	Not Reported	Ground						24 954.6		12
		Not Reported	Ground						24 977.	5.	19
		Not Reported	Ground						24 997.	5.	19
		Not Reported	Ground						25 017.8		12
		Not Reported	Ground						25 050.	5.	12
		Not Reported	Ground						25 056.31	.1	37
		Not Reported	Ground						25 131.	5.	19
		Not Reported	Ground						25 151.	5.	19
		Not Reported	Ground						25 289.	5.	19
		Not Reported	Ground						25 300.3		12
		Not Reported	Ground						25 312.	5.	19
		Not Reported	Ground						25 322.98	.1	37
		Not Reported	Ground						25 332.	5.	19
		Not Reported	Ground						25 349.	5.	19
		Not Reported	Ground						25 385.	5.	12
		Not Reported	Ground						25 796.	5.	12
		Not Reported	Ground						25 898.	5.	12
		Not Reported	Ground						26 120.50	.1	37
		Not Reported	Ground						26 550.15	.1	37
		Not Reported	Ground						26 562.	5.	12
		Not Reported	Ground						26 778.9	.1	37
		Not Reported	Ground						26 783.18	.1	37
		Not Reported	Ground						26 854.		13
		Not Reported	Ground						27 227.02	.1	37
		Not Reported	Ground						27 283.29	.1	37
		Not Reported	Ground						27 450.		13
		Not Reported	Ground						27 700.1	.1	37
		Not Reported	Ground						27 817.50	.1	37
		Not Reported	Ground						27 820.87	.1	37
		Not Reported	Ground						28 119.5	.1	37
		Not Reported	Ground						28 500.		13
		Not Reported	Ground						28 550.		13
		Not Reported	Ground						28 969.9	.1	37
		Not Reported	Ground						29 113.76	.1	37
		Not Reported	Ground						29 889.33	.1	37
		Not Reported	Ground						29 950.		13
		Not Reported	Ground						30 678.66	.1	37
		Not Reported	Ground						30 693.42	.1	37
		Not Reported	Ground						31 673.05	.1	37
		Not Reported	Ground						31 757.42	.1	37
		Not Reported	Ground						31 977.82	.1	37
		Not Reported	Ground						32 379.37	.1	37
		Not Reported	Ground						32 398.44	.1	37
		Not Reported	Ground						33 089.91	.1	37
		Not Reported	Ground						33 414.1	.1	37
		Not Reported	Ground						33 566.20	.1	37
		Not Reported	Ground						33 568.2	.1	37
		Not Reported	Ground						33 691.63	.1	37
		Not Reported	Ground						33 693.74	.1	37
		Not Reported	Ground						34 001.35	.1	37

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3O^{16}H$	211	Not Reported	Ground							34 003.69	.1	37
		Not Reported	Ground							34 236.91	.1	37
		Not Reported	Ground							34 417.86	.1	37
		Not Reported	Ground							35 161.6	.1	37
		Not Reported	Ground							35 478.55	.1	37
		Not Reported	Ground							35 738.32	.1	37
		Not Reported								36 240.		396
		Not Reported	Ground							36 248.14	.1	37
		Not Reported	Ground							37 044.68	.1	37
		Not Reported								37 690.		396
		Not Reported								38 290.		396
		Not Reported								38 335.		396
		Not Reported								38 445.		396
		Not Reported								42 280.		396
		Not Reported								44 100.		396
		Not Reported								46 610.		396
		Not Reported								47 870.		396
		Not Reported								48 010.		396
		Not Reported								48 260.		396
		Not Reported								48 406.		396
		Not Reported								48 707.7		396
		Not Reported								49 032.		396
		Not Reported								49 750.		396
$C^{12}H_3O^{16}D$	212	1, 0, 1← 0, 0, 0	Ground	A	2					45 189.46	1.0	121
		1, 0, 1← 0, 0, 0	Ground	E	2					45 193.36	1.0	121
		1, 0, 1← 0, 0, 0	Ground	E	1					45 259.44	1.	121
		1, 0, 1← 0, 0, 0	Ground	A	1					45 265.78	1.	121
		1, 0, 1← 0, 0, 0	Ground	A	0					45 344.30	1.	121
		1, 0, 1← 0, 0, 0	Ground	E	0					45 359.43	1.	121
		1, 0, 1← 0, 0, 0								47 359.7		396
		Not Reported								47 052.		396
		Not Reported								47 266.		396
		Not Reported								47 346.		396
$C^{13}H_3O^{16}H$	213	1, 0, 1← 0, 0, 0	Ground	A	2					47 019.5	1.0	121
		1, 0, 1← 0, 0, 0	Ground	E	2					47 030.16	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	1					47 083.82	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	1					47 094.11	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	0					47 205.20	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	0					47 209.63	.5	121
		1, 0, 1← 0, 0, 0								48 529.6		396
		2, 2, ← 2, 1,	Ground	E(–)	0					27 052.97	.1	37
		3, 2, ← 3, 1,	Ground	E(–)	0					27 047.19	.1	37
		4, 2, ← 4, 1,	Ground	E(–)	0					27 050.45	.1	37
		5, 2, ← 5, 1,	Ground	E(–)	0					27 072.17	.1	37
		6, 2, ← 6, 1,	Ground	E(–)	0					27 122.76	.1	37
		7, 2, ← 7, 1,	Ground	E(–)	0					27 215.60	.1	37
		8, 2, ← 8, 1,	Ground	E(–)	0					27 364.12	.1	37
		9, 2, ← 9, 1,	Ground	E(–)	0					27 581.65	.1	37
		10, 2, ←10, 1,	Ground	E(–)	0					27 880.04	.1	37

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_3O^{16}H$	213	11, 2, ←11, 1,	Ground	E(−)	0					28 267.71	.1	37
		12, 2, ←12, 1,	Ground	E(−)	0					28 747.67	.1	37
		13, , ←12, ,	Ground							26 979.03	.1	37
		13, , ←12, ,	Ground							26 980.40	.1	37
		13, , ←12, ,	Ground							27 104.80	.1	37
		13, , ←12, ,	Ground							27 105.93	.1	37
		13, 2, ←13, 1,	Ground	E(−)	0					29 315.20	.1	37
		14, 2, ←14, 1,	Ground	E(−)	0					29 955.72	.1	37
		15, 2, ←15, 1,	Ground	E(−)	0					30 643.69	.1	37
		16, 2, ←16, 1,	Ground	E(−)	0					31 342.31	.1	37
		17, 2, ←17, 1,	Ground	E(−)	0					32 004.43	.1	37
		18, 2, ←18, 1,	Ground	E(−)	0					32 575.53	.1	37
		19, 2, ←19, 1,	Ground	E(−)	0					32 998.94	.1	37
		20, 2, ←20, 1,	Ground	E(−)	0					33 220.05	.1	37
		21, 2, ←21, 1,	Ground	E(−)	0					33 192.97	.1	37
		22, 2, ←22, 1,	Ground	E(−)	0					32 883.47	.1	37
		23, 2, ←23, 1,	Ground	E(−)	0					32 271.10	.1	37
		24, 2, ←24, 1,	Ground	E(−)	0					31 350.19	.1	37
		25, 2, ←25, 1,	Ground	E(−)	0					30 127.80	.1	37
		26, 2, ←26, 1,	Ground	E(−)	0					28 621.04	.1	37
		27, 2, ←27, 1,	Ground	E(−)	0					26 855.01	.1	37
		28, 2, ←28, 1,	Ground	E(−)	0					24 860.62	.1	37
		29, 2, ←29, 1,	Ground	E(−)	0					22 672.90	.1	37
		30, 2, ←30, 1,	Ground	E(−)	0					20 329.32	.1	37
		31, 2, ←31, 1,	Ground	E(−)	0					17 870.5	.1	37
		Not Reported	Ground							28 869.59	.1	37
		Not Reported								47 080.		396
		Not Reported								47 760.		396
		Not Reported								47 899.3		396
		Not Reported								47 950.1		396
		Not Reported								49 070.8		396
$C^{12}D_3O^{16}H$	214	1, 0, 1← 0, 0, 0	Ground	A	2					38 923.97	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	2					38 928.89	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	1					38 972.05	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	1					38 982.88	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	0					39 066.21	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	0					39 069.25	.5	121
		2, , ← 1, ,	Ground							37 229.8	.5	121
		2, , ← 1, ,	Ground							40 649.5	.5	121
		2, , ← 1, ,	Ground							43 453.7	.5	121
		4, , ← 3, ,	Ground							35 748.2	.5	121
		5, , ← 4, ,	Ground							43 501.5	.5	121
		Not Reported	Ground							17 775.1	.5	121
		Not Reported	Ground							17 839.1	.5	121
		Not Reported	Ground							17 918.9	.5	121
		Not Reported	Ground							18 081.2	.5	121
		Not Reported	Ground							18 097.0	.5	121
		Not Reported	Ground							18 227.3	.5	121
		Not Reported	Ground							18 395.6	.5	121

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3O^{16}H$	214	Not Reported	Ground							18 588.6	.5	121
		Not Reported	Ground							18 796.2	.5	121
		Not Reported	Ground							18 923.7	.5	121
		Not Reported	Ground							19 294.5	.5	121
		Not Reported	Ground							19 844.8	.5	121
		Not Reported	Ground							19 905.8	.5	121
		Not Reported	Ground							20 469.8	.5	121
		Not Reported	Ground							20 642.5	.5	121
		Not Reported	Ground							21 236.4	.5	121
		Not Reported	Ground							21 519.5	.5	121
		Not Reported	Ground							22 174.1	.5	121
		Not Reported	Ground							22 550.3	.5	121
		Not Reported	Ground							23 313.9	.5	121
		Not Reported	Ground							23 750.0	.5	121
		Not Reported	Ground							24 691.9	.5	121
		Not Reported	Ground							25 133.2	.5	121
		Not Reported	Ground							26 344.7	.5	121
		Not Reported	Ground							26 715.3	.5	121
		Not Reported	Ground							27 982.7	.5	121
		Not Reported	Ground							28 032.7	.5	121
		Not Reported	Ground							28 311.9	.5	121
		Not Reported	Ground							28 511.7	.5	121
		Not Reported	Ground							35 805.7	.5	121
		Not Reported	Ground							35 810.8	.5	121
		Not Reported	Ground							36 332.7	.5	121
		Not Reported	Ground							36 422.9	.5	121
		Not Reported	Ground							36 483.9	.5	121
		Not Reported	Ground							36 663.0	.5	121
		Not Reported	Ground							37 322.8	.5	121
		Not Reported	Ground							37 462.6	.5	121
		Not Reported	Ground							37 900.0	.5	121
		Not Reported	Ground							38 052.6	.5	121
		Not Reported	Ground							38 132.8	.5	121
		Not Reported	Ground							38 967.6	.5	121
		Not Reported	Ground							40 229.8	.5	121
		Not Reported	Ground							41 684.6	.5	121
		Not Reported	Ground							42 163.8	.5	121
		Not Reported	Ground							42 292.1	.5	121
		Not Reported	Ground							43 325.0	.5	121
$C^{13}H_3O^{16}D$	215	1, 0, 1← 0, 0, 0	Ground	A	2					44 076.55	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	2					44 079.30	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	1					44 144.06	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	1					44 151.09	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	0					44 228.26	.5	121
		1, 0, 1← 0, 0, 0	Ground	E	0					44 241.43	.5	121
$C^{12}D_3O^{16}D$	216	1, 0, 1← 0, 0, 0	Ground	A	2					36 673.93	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	1					36 730.94	.5	121
		1, 0, 1← 0, 0, 0	Ground	A	0					36 799.01	.5	121
		Not Reported								30 505.		396

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3O^{16}D$	216	Not Reported							30 600.		396
		Not Reported							31 140.		396
		Not Reported							32 190.		396
		Not Reported							32 325.		396
		Not Reported							32 790.		396
		Not Reported							33 340.		396
		Not Reported							33 965.		396
		Not Reported							34 410.		396
		Not Reported							35 090.		396
		Not Reported							35 100.		396
		Not Reported							35 165.		396
		Not Reported							35 215.		396
		Not Reported							35 335.		396
		Not Reported							35 440.		396
		Not Reported							35 748.2		396
		Not Reported							35 805.7		396
		Not Reported							35 810.8		396
		Not Reported							36 080.0		396
		Not Reported							36 332.7		396
		Not Reported							36 422.9		396
		Not Reported							36 483.9		396
		Not Reported							36 655.		396
		Not Reported							36 946.4		396
		Not Reported							36 987.		396
		Not Reported							37 030.		396
		Not Reported							37 229.8		396
		Not Reported							37 322.8		396
		Not Reported							37 325.		396
		Not Reported							37 425.		396
		Not Reported							37 462.6		396
		Not Reported							37 900.		396
		Not Reported							38 052.6		396
		Not Reported							38 132.8		396
		Not Reported							38 530.		396
		Not Reported							38 967.0		396
		Not Reported							39 048.		396
		Not Reported							39 065.		396
		Not Reported							40 083.		396
		Not Reported							40 240.		396
		Not Reported							40 640.		396
		Not Reported							40 940.		396
		Not Reported							41 230.		396
		Not Reported							41 540.		396
		Not Reported							41 688.		396
		Not Reported							41 750.		396
		Not Reported							42 000.		396
		Not Reported							42 020.		396
		Not Reported							42 150.		396
		Not Reported							42 285.		396
		Not Reported							42 700.		396

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3O^{16}D$	216	Not Reported								43 345.		396
		Not Reported								43 525.		396
		Not Reported								43 545.		396
		Not Reported								43 630.		396
		Not Reported								43 995.		396
$C^{12}H_3O^{18}H$	217	2, 2, ← 2, 1,	Ground	E(−)	0					33 918.97	.1	37
		3, 2, ← 3, 1,	Ground	E(−)	0					33 925.49	.1	37
		4, 2, ← 4, 1,	Ground	E(−)	0					33 943.63	.1	37
		5, 2, ← 5, 1,	Ground	E(−)	0					33 981.35	.1	37
		6, 2, ← 6, 1,	Ground	E(−)	0					34 048.42	.1	37
		7, 2, ← 7, 1,	Ground	E(−)	0					34 155.63	.1	37
		8, 2, ← 8, 1,	Ground	E(−)	0					34 314.64	.1	37
		9, 2, ← 9, 1,	Ground	E(−)	0					34 536.74	.1	37
		10, 2, ←10, 1,	Ground	E(−)	0					34 831.64	.1	37
		11, 2, ←11, 1,	Ground	E(−)	0					35 206.11	.1	37
		12, 2, ←12, 1,	Ground	E(−)	0					35 661.78	.1	37
		13, 2, ←13, 1,	Ground	E(−)	0					36 193.55	.1	37
		14, 2, ←14, 1,	Ground	E(−)	0					36 787.33	.1	37
		15, 2, ←15, 1,	Ground	E(−)	0					37 418.97	.1	37
		16, 2, ←16, 1,	Ground	E(−)	0					38 053.87	.1	37
		17, 2, ←17, 1,	Ground	E(−)	0					38 647.87	.1	37
		18, 2, ←18, 1,	Ground	E(−)	0					39 149.41	.1	37
		19, 2, ←19, 1,	Ground	E(−)	0					39 505.01	.1	37
		20, 2, ←20, 1,	Ground	E(−)	0					39 661.80	.1	37
		21, 2, ←21, 1,	Ground	E(−)	0					39 574.97	.1	37
		22, 2, ←22, 1,	Ground	E(−)	0					39 210.48	.1	37
		23, 2, ←23, 1,	Ground	E(−)	0					38 547.73	.1	37
		24, 2, ←24, 1,	Ground	E(−)	0					37 579.85	.1	37
		25, 2, ←25, 1,	Ground	E(−)	0					36 312.57	.1	37
		26, 2, ←26, 1,	Ground	E(−)	0					34 761.75	.1	37

CH_4S $C_s(C_{3v},C_s)$ CH_3SH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3S^{32}H$	C_s	221	170 303. M	12 907.36 M	12 384.04 M				
$C^{13}H_3S^{32}H$	C_s	222	170 296. M	12 433.73 M	11 947.34 M				
$C^{12}H_3S^{32}D$	C_s	223	91 026. M	12 659.24 M	11 727.55 M				
$C^{12}D_3S^{32}H$	C_s	224	120 849. M	10 541.56 M	10 189.68 M				
$C^{12}H_3S^{34}H$	C_s	225	170 016. M	12 694.62 M	12 186.94 M				
$C^{12}H_3S^{33}H$	C_s	226	170 155. M	12 797.80 M	12 282.55 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
221	1.33 M	0.73 M	0. X		1270	1.0					

References:

ABC: 106 D_J: D_{JK}: κ: Δ:

μ: 286 eQq: V: 344 I: ω:

Add. Refs.: 38, 47, 84, 107, 141', 164

Torsional frequency = 200 cm^{-1}. Ref: 286. $eQq_{aa} = -27.57 \pm .05$ MHz. Ref: 383.

Methanethiol

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3S^{32}H$	221	1, 0, 1← 0, 0, 0	Ground	A	3					25 126.9	.1	174
		1, 0, 1← 0, 0, 0	Ground	E	3					25 142.2	.1	174
		1, 0, 1← 0, 0, 0	Ground	A	2					25 143.6	.1	174
		1, 0, 1← 0, 0, 0	Ground	E	2					25 154.8	.1	174
		1, 0, 1← 0, 0, 0	Ground	E	1					25 206.8	.1	174
		1, 0, 1← 0, 0, 0	Ground	A	1					25 219.7	.1	174
		1, 0, 1← 0, 0, 0	Ground	A	0					25 290.8	.1	174
		1, 0, 1← 0, 0, 0	Ground	E	0					25 291.8	.1	174
		1, 1, ← 2, 0,	Ground	E(+)	0					14 764.5	.1	174
		2, 1, ← 1, 0,	Ground	E(+)	1					18 417.6		286
		2, 1, ← 3, 0,	Ground	E(−)	0					23 339.2	.1	174
		2, 1, 2← 3, 0, 3	Ground	A	0					29 091.9	.1	174
		3, 2, 1← 2, 1, 2	Ground	A	1					15 339.0		286
		3, 2, 2← 2, 1, 1	Ground	A	1					14 320.2		286
		4, 0, ← 3, 1,	Ground							35 857.4		286
		5, 0, ← 4, 1,	Ground	E(−)	0					26 994.2	.1	174
		5, 0, 5← 4, 1, 4	Ground	A	0					23 256.9	.1	174
		5, 1, 4← 5, 1, 5	Ground							7 846.0	.1	174
		6, 1, 5← 6, 1, 6	Ground							10 983.4	.1	174
		7, 1, 6← 7, 1, 7	Ground							14 643.1	.1	174

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3S^{32}H$	221	8, 1, 7← 8, 1, 8	Ground							18 824.2	.1	174
		8, 2, ← 9, 1,	Ground	E(–)	0					18 039.5	.1	174
		9, 1, 8← 9, 1, 9	Ground							23 526.2	.1	174
		9, 2, ←10, 1,	Ground							21 973.2		286
		9, 2, 8←10, 1, 9	Ground	A	0					25 659.7	.1	174
		10, 1, 9←10, 1,10	Ground							28 747.9	.1	174
		10, 2, 8←11, 1,11	Ground							33 077.9		286
		11, 1, ←10, 2,	Ground							35 913.5		286
		12, 1, ←11, 2,	Ground							23 801.8		286
		12, 1,11←11, 2,10	Ground							30 741.8		286
		14, 1,14←13, 2,11	Ground							30 508.6		286
		Not Reported	Ground							14 146.3	.1	174
		Not Reported	Ground							14 548.4	.1	174
		Not Reported	Ground							14 865.1	.1	174
		Not Reported	Ground							14 888.0	.1	174
		Not Reported	Ground							15 089.3	.1	174
		Not Reported	Ground							15 102.2	.1	174
		Not Reported	Ground							15 103.5	.1	174
		Not Reported	Ground							15 123.2	.1	174
		Not Reported	Ground							15 165.1	.1	174
		Not Reported	Ground							15 335.9	.1	174
		Not Reported	Ground							16 057.0	.1	174
		Not Reported	Ground							16 059.8	.1	174
		Not Reported	Ground							16 066.1	.1	174
		Not Reported	Ground							16 796.4	.1	174
		Not Reported	Ground							17 320.4	.1	174
		Not Reported	Ground							18 257.8	.1	174
		Not Reported	Ground							18 396.0	.1	174
		Not Reported	Ground							18 431.8	.1	174
		Not Reported	Ground							18 446.3	.1	174
		Not Reported	Ground							18 494.1	.1	174
		Not Reported	Ground							18 499.7	.1	174
		Not Reported	Ground							18 509.7	.1	174
		Not Reported	Ground							18 586.1	.1	174
		Not Reported	Ground							18 675.6	.1	174
		Not Reported	Ground							18 778.6	.1	174
		Not Reported	Ground							18 806.4	.1	174
		Not Reported	Ground							18 895.7	.1	174
		Not Reported	Ground							18 991.8	.1	174
		Not Reported	Ground							19 027.1	.1	174
		Not Reported	Ground							19 173.0	.1	174
		Not Reported	Ground							19 273.6	.1	174
		Not Reported	Ground							19 334.0	.1	174
		Not Reported	Ground							19 510.4	.1	174
		Not Reported	Ground							19 568.3	.1	174
		Not Reported	Ground							19 702.9	.1	174
		Not Reported	Ground							19 912.2	.1	174
		Not Reported	Ground							19 999.9	.1	174
		Not Reported	Ground							20 052.6	.1	174
		Not Reported	Ground							20 138.6	.1	174
		Not Reported	Ground							20 241.9	.1	174
		Not Reported,	Ground							20 383.2	.1	174
		Not Reported	Ground							20 646.4	.1	174
		Not Reported	Ground							20 928.9	.1	174
		Not Reported	Ground							21 057.4	.1	174

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3S^{32}H$	221	Not Reported	Ground						21 131.1	.1	174
		Not Reported	Ground						21 231.7	.1	174
		Not Reported	Ground						21 519.9	.1	174
		Not Reported	Ground						21 555.6	.1	174
		Not Reported	Ground						21 734.6	.1	174
		Not Reported	Ground						21 766.6	.1	174
		Not Reported	Ground						21 865.5	.1	174
		Not Reported	Ground						21 877.1	.1	174
		Not Reported	Ground						21 901.0	.1	174
		Not Reported	Ground						21 943.5	.1	174
		Not Reported	Ground						22 269.4	.1	174
		Not Reported	Ground						22 329.8	.1	174
		Not Reported	Ground						22 560.2	.1	174
		Not Reported	Ground						22 661.4	.1	174
		Not Reported	Ground						22 827.3	.1	174
		Not Reported	Ground						23 073.8	.1	174
		Not Reported	Ground						23 078.2	.1	174
		Not Reported	Ground						23 230.3	.1	174
		Not Reported	Ground						23 494.4	.1	174
		Not Reported	Ground						23 520.4	.1	174
		Not Reported	Ground						23 566.6	.1	174
		Not Reported	Ground						23 617.3	.1	174
		Not Reported	Ground						23 773.8	.1	174
		Not Reported	Ground						23 989.0	.1	174
		Not Reported	Ground						24 067.5	.1	174
		Not Reported	Ground						24 485.0	.1	174
		Not Reported	Ground						24 988.5	.1	174
		Not Reported	Ground						25 009.0	.1	174
		Not Reported	Ground						25 121.4	.1	174
		Not Reported	Ground						25 562.0	.1	174
		Not Reported	Ground						25 917.5	.1	174
		Not Reported	Ground						26 077.4	.1	174
		Not Reported	Ground						26 144.7	.1	174
		Not Reported	Ground						26 388.4	.1	174
		Not Reported	Ground						26 758.1	.1	174
		Not Reported	Ground						26 947.0	.1	174
		Not Reported	Ground						27 235.8	.1	174
		Not Reported	Ground						27 333.9	.1	174
		Not Reported	Ground						27 364.5	.1	174
		Not Reported	Ground						27 402.2	.1	174
		Not Reported	Ground						27 419.4	.1	174
		Not Reported	Ground						27 444.5	.1	174
		Not Reported	Ground						27 911.9	.1	174
		Not Reported	Ground						28 078.2	.1	174
		Not Reported	Ground						28 275.1	.1	174
		Not Reported	Ground						28 530.1	.1	174
		Not Reported	Ground						28 593.5	.1	174
		Not Reported	Ground						28 686.8	.1	174
		Not Reported	Ground						28 786.0	.1	174
		Not Reported	Ground						28 910.8	.1	174
		Not Reported	Ground						28 990.3	.1	174
		Not Reported	Ground						29 073.9	.1	174
		Not Reported	Ground						29 074.4	.1	174
		Not Reported	Ground						29 436.3	.1	174
		Not Reported	Ground						29 526.2	.1	174

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3S^{32}H$	221	Not Reported	Ground						29 574.4	.1	174
		Not Reported	Ground						29 593.1	.1	174
		Not Reported	Ground						29 772.81		286
		Not Reported	Ground						30 083.34		286
		Not Reported	Ground						30 366.66		286
		Not Reported	Ground						30 395.6		286
		Not Reported	Ground						30 446.3		286
		Not Reported	Ground						30 487.4		286
		Not Reported	Ground						30 626.50		286
		Not Reported	Ground						30 652.31		286
		Not Reported	Ground						30 666.43		286
		Not Reported	Ground						30 859.78		286
		Not Reported	Ground						30 874.84		286
		Not Reported	Ground						30 972.32		286
		Not Reported	Ground						31 051.0		286
		Not Reported	Ground						31 068.24		286
		Not Reported	Ground						31 252.87		286
		Not Reported	Ground						31 378.7		286
		Not Reported	Ground						31 414.80		286
		Not Reported	Ground						31 450.2		286
		Not Reported	Ground						31 476.5		286
		Not Reported	Ground						31 479.3		286
		Not Reported	Ground						31 489.3		286
		Not Reported	Ground						31 496.2		286
		Not Reported	Ground						31 500.8		286
		Not Reported	Ground						31 522.7		286
		Not Reported	Ground						31 527.2		286
		Not Reported	Ground						31 529.9		286
		Not Reported	Ground						31 540.4		286
		Not Reported	Ground						31 555.09		286
		Not Reported	Ground						31 563.8		286
		Not Reported	Ground						31 567.9		286
		Not Reported	Ground						31 571.8		286
		Not Reported	Ground						31 575.4		286
		Not Reported	Ground						31 675.02		286
		Not Reported	Ground						31 776.04		286
		Not Reported	Ground						31 859.54		286
		Not Reported	Ground						31 880.2		286
		Not Reported	Ground						31 927.27		286
		Not Reported	Ground						31 980.68		286
		Not Reported	Ground						31 989.58		286
		Not Reported	Ground						31 994.74		286
		Not Reported	Ground						32 002.23		286
		Not Reported	Ground						32 011.70		286
		Not Reported	Ground						32 021.14		286
		Not Reported	Ground						32 022.71		286
		Not Reported	Ground						32 034.82		286
		Not Reported	Ground						32 047.20		286
		Not Reported	Ground						32 050.46		286
		Not Reported	Ground						32 059.35		286
		Not Reported	Ground						32 070.04		286
		Not Reported	Ground						32 070.15		286
		Not Reported	Ground						32 078.93		286
		Not Reported	Ground						32 081.32		286
		Not Reported	Ground						32 084.51		286

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3S^{32}H$	221	Not Reported	Ground						32 085.74		286
		Not Reported	Ground						32 278.04		286
		Not Reported	Ground						32 819.24		286
		Not Reported	Ground						32 820.71		286
		Not Reported	Ground						32 827.91		286
		Not Reported	Ground						32 844.33		286
		Not Reported	Ground						32 874.34		286
		Not Reported	Ground						32 880.05		286
		Not Reported	Ground						32 922.31		286
		Not Reported	Ground						32 994.15		286
		Not Reported	Ground						33 095.66		286
		Not Reported	Ground						33 096.66		286
		Not Reported	Ground						33 233.51		286
		Not Reported	Ground						33 277.30		286
		Not Reported	Ground						33 414.78		286
		Not Reported	Ground						33 416.85		286
		Not Reported	Ground						33 647.20		286
		Not Reported	Ground						33 658.81		286
		Not Reported	Ground						33 738.45		286
		Not Reported	Ground						33 838.93		286
		Not Reported	Ground						33 858.74		286
		Not Reported	Ground						33 938.69		286
		Not Reported	Ground						34 013.70		286
		Not Reported	Ground						34 193.09		286
		Not Reported	Ground						34 237.2		286
		Not Reported	Ground						34 298.00		286
		Not Reported	Ground						34 488.25		286
		Not Reported	Ground						34 527.38		286
		Not Reported	Ground						34 616.85		286
		Not Reported	Ground						34 733.89		286
		Not Reported	Ground						34 942.56		286
		Not Reported	Ground						35 255.73		286
		Not Reported	Ground						35 373.8		286
		Not Reported	Ground						35 521.54		286
		Not Reported	Ground						35 543.34		286
		Not Reported	Ground						35 547.33		286
		Not Reported	Ground						35 552.2		286
		Not Reported	Ground						35 597.59		286
		Not Reported	Ground						35 731.0		286
		Not Reported	Ground						35 754.19		286
		Not Reported	Ground						35 791.03		286
		Not Reported	Ground						35 792.1		286
		Not Reported	Ground						35 846.05		286
		Not Reported	Ground						35 873.42		286
		Not Reported	Ground						35 924.22		286
		Not Reported	Ground						36 026.20		286
		Not Reported	Ground						36 030.87		286
		Not Reported	Ground						36 172.20		286
		Not Reported	Ground						36 216.46		286
		Not Reported	Ground						36 281.75		286
		Not Reported	Ground						36 354.69		286
		Not Reported	Ground						36 585.17		286
		Not Reported	Ground						36 597.09		286
		Not Reported	Ground						36 822.40		286
		Not Reported	Ground						36 824.83		286
		Not Reported	Ground						36 871.10		286
		Not Reported	Ground						37 220.42		286
		Not Reported	Ground						37 437.33		286

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_3S^{32}H$	222	1, 0, 1← 0, 0, 0	Ground	A	2					24 245.0		174
		1, 0, 1← 0, 0, 0	Ground	E	2					24 256.2		174
		1, 0, 1← 0, 0, 0	Ground	E	1					24 306.2		174
		1, 0, 1← 0, 0, 0	Ground	A	1					24 318.5		174
		1, 0, 1← 0, 0, 0	Ground	E	0					24 388.0		174
		1, 0, 1← 0, 0, 0	Ground	A	0					24 389.1		174
$C^{12}H_3S^{32}D$	223	1, 0, 1← 0, 0, 0	Ground	A	3					24 302.9		174
		1, 0, 1← 0, 0, 0	Ground	A	2					24 322.2		174
		1, 0, 1← 0, 0, 0	Ground	E	2					24 330.3		174
		1, 0, 1← 0, 0, 0	Ground	E	1					24 385.9		174
		1, 0, 1← 0, 0, 0	Ground	A	1					24 388.3		174
		1, 0, 1← 0, 0, 0	Ground	A	0					24 456.0		174
$C^{12}D_3S^{32}H$	224	1, 0, 1← 0, 0, 0	Ground	A	2					20 619.0		174
		1, 0, 1← 0, 0, 0	Ground	E	2					20 627.6		174
		1, 0, 1← 0, 0, 0	Ground	E	1					20 674.8		174
		1, 0, 1← 0, 0, 0	Ground	A	1					20 678.9		174
		1, 0, 1← 0, 0, 0	Ground	A	0					20 732.0		174
		1, 0, 1← 0, 0, 0	Ground	E	0					20 732.8		174
$C^{12}H_3S^{34}H$	225	1, 0, 1← 0, 0, 0	Ground							24 878.9		119
		1, 0, 1← 0, 0, 0	Ground							24 879.8		119
$C^{12}H_3S^{33}H$	226	1, 0, 1← 0, 0, 0	Ground							25 078.7		119
		1, 0, 1← 0, 0, 0	Ground							25 079.6		119

CH_5ClSi $C_s(C_{3v},C_s)$ CH_2ClSiH_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_2Cl^{35}Si^{28}H_3$	C_s	231	21 759.21 M	3 204.08 M	2 938.09 M	.004			
$C^{12}H_2Cl^{37}Si^{28}H_3$	C_s	232	21 692.92 M	3 125.14 M	2 870.40 M				
$C^{13}H_2Cl^{35}Si^{28}H_3$	C_s	233	21 080.42 M	3 204.37 M	2 925.47 M				
$C^{12}H_2Cl^{35}Si^{29}H_3$	C_s	234	21 726.82 M	3 155.41 M	2 896.53 M				
$C^{12}D_2Cl^{35}Si^{28}H_3$	C_s	235	17 282.73 M	3 172.57 M	2 864.21 M				
$C^{12}HDCl^{35}Si^{28}H_3$	C_1	236	19 250.99 M	3 190.78 M	2 898.44 M				
$C^{12}H_2Cl^{35}Si^{28}D_3$	C_s	237	17 536.11 M	2 925.97 M	2 707.51 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
231				−32.51	2550	50					

References:

ABC: 358 D_J: 358 D_{JK}: κ: Δ:

eQq: 358 V: 358 I: ω:

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2Cl^{35}Si^{28}H_3$	231	4, 0, 4← 3, 0, 3	Ground							24 539.45	.2	358
		4, 1, 3← 3, 1, 2	Ground							25 093.48	.2	358
		4, 1, 4← 3, 1, 3	Ground							24 030.18	.2	358
		5, 0, 5← 4, 0, 4	Ground		1					30 517.53	.2	358
		5, 0, 5← 4, 0, 4	Ground							30 652.24	.2	358
		5, 1, 4← 4, 1, 3	Ground		1					31 203.74	.2	358
		5, 1, 4← 4, 1, 3	Ground							31 360.87	.2	358
		5, 1, 5← 4, 1, 4	Ground		1					29 915.57	.2	358
		5, 1, 5← 4, 1, 4	Ground							30 032.34	.2	358
		5, 1, 4← 5, 0, 5	Ground				7/2		7/2	20 757.70	.2	358
		5, 1, 4← 5, 0, 5	Ground				13/2		13/2	20 759.47	.2	358
		5, 1, 4← 5, 0, 5	Ground							20 761.87	.2	358
		5, 1, 4← 5, 0, 5	Ground				9/2		9/2	20 763.92	.2	358
		5, 1, 4← 5, 0, 5	Ground				11/2		11/2	20 765.66	.2	358
		6, 1, 5← 6, 0, 6	Ground				9/2		9/2	21 631.36	.2	358
		6, 1, 5← 6, 0, 6	Ground				15/2		15/2	21 632.81	.2	358
		6, 1, 5← 6, 0, 6	Ground							21 634.98	.2	358
		6, 1, 5← 6, 0, 6	Ground				11/2		11/2	21 637.41	.2	358
		6, 1, 5← 6, 0, 6	Ground				13/2		13/2	21 638.88	.2	358
		7, 1, 6← 7, 0, 7	Ground		1					22 477.10	.2	358
		7, 1, 6← 7, 0, 7	Ground				11/2		11/2	22 681.16	.2	358
		7, 1, 6← 7, 0, 7	Ground				17/2		17/2	22 682.47	.2	358
		7, 1, 6← 7, 0, 7	Ground							22 684.78	.2	358
		7, 1, 6← 7, 0, 7	Ground				13/2		13/2	22 687.29	.2	358
		7, 1, 6← 7, 0, 7	Ground				15/2		15/2	22 688.51	.2	358
		8, 1, 7← 8, 0, 8	Ground		1					23 674.57	.2	358
		8, 1, 7← 8, 0, 8	Ground				13/2		13/2	23 920.73	.2	358
		8, 1, 7← 8, 0, 8	Ground				19/2		19/2	23 921.78	.2	358
		8, 1, 7← 8, 0, 8	Ground							23 924.41	.2	358
		8, 1, 7← 8, 0, 8	Ground				15/2		15/2	23 926.95	.2	358
		8, 1, 7← 8, 0, 8	Ground				17/2		17/2	23 927.90	.2	358
		9, 1, 8← 9, 0, 9	Ground				15/2		15/2	25 364.62	.2	358
		9, 1, 8← 9, 0, 9	Ground				21/2		21/2	25 365.55	.2	358
		9, 1, 8← 9, 0, 9	Ground							25 368.30	.2	358
		9, 1, 8← 9, 0, 9	Ground				17/2		17/2	25 370.91	.2	358
		9, 1, 8← 9, 0, 9	Ground				19/2		19/2	25 371.91	.2	358
		9, 3, 6←10, 2, 9	Ground	A	1					32 233.43	.2	358 [1]
		9, 3, 6←10, 2, 9	Ground	E	1					32 234.65	.2	358 [1]
		9, 3, 6←10, 2, 9	Ground	A	1					32 235.62	.2	358 [1]
		9, 3, 6←10, 2, 9	Ground	E	1					32 236.82	.2	358 [1]
		9, 3, 7←10, 2, 8	Ground	A	1					30 914.77	.2	358
		9, 3, 7←10, 2, 8	Ground	E	1					30 915.52	.2	358
		10, 1, 9←10, 0,10	Ground		1					26 672.38	.2	358
		10, 1, 9←10, 0,10	Ground				17/2		17/2	27 027.28	.2	358
		10, 1, 9←10, 0,10	Ground				23/2		23/2	27 028.20	.2	358
		10, 1, 9←10, 0,10	Ground							27 031.04	.2	358
		10, 1, 9←10, 0,10	Ground				19/2		19/2	27 033.77	.2	358
		10, 1, 9←10, 0,10	Ground				21/2		21/2	27 034.75	.2	358
		10, 3, 7←11, 2,10	Ground	A	1					26 282.6	.2	358 [1]
		10, 3, 7←11, 2,10	Ground	E	1					26 283.9	.2	358 [1]

1. The two sets of numbers given for two of the transitions in the first excited torsional state are a result of the partially resolved hyperfine structure due to quadrupole coupling.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2Cl^{35}Si^{28}H_3$	231	10, 3, 7←11, 2,10	Ground	A	1					26 284.7	.2	358 [1]
		10, 3, 7←11, 2,10	Ground	E	1					26 285.8	.2	358 [1]
		10, 3, 8←11, 2, 9	Ground	A	1					24 383.97	.2	358
		10, 3, 8←11, 2, 9	Ground	E	1					24 384.93	.2	358
		11, 1,10←11, 0,11	Ground		1					28 501.29	.2	358
		11, 1,10←11, 0,11	Ground				19/2		19/2	28 923.43	.2	358
		11, 1,10←11, 0,11	Ground				25/2		25/2	28 924.30	.2	358
		11, 1,10←11, 0,11	Ground							28 927.25	.2	358
		11, 1,10←11, 0,11	Ground				21/2		21/2	28 930.08	.2	358
		11, 1,10←11, 0,11	Ground				23/2		23/2	28 931.01	.2	358
		12, 1,11←12, 0,12	Ground				21/2		21/2	31 066.54	.2	358
		12, 1,11←12, 0,12	Ground				27/2		27/2	31 067.32	.2	358
		12, 1,11←12, 0,12	Ground							31 070.41	.2	358
		12, 1,11←12, 0,12	Ground				23/2		23/2	31 073.42	.2	358
		12, 1,11←12, 0,12	Ground				25/2		25/2	31 074.25	.2	358
$C^{12}H_2Cl^{37}Si^{28}H_3$	232	4, 0, 4← 3, 0, 3	Ground							23 955.17	.2	358
		4, 1, 3← 3, 1, 2	Ground							24 485.10	.2	358
		4, 1, 4← 3, 1, 3	Ground							23 466.80	.2	358
		5, 0, 5← 4, 0, 4	Ground							29 923.80	.2	358
		5, 1, 4← 4, 1, 3	Ground							30 601.08	.2	358
		6, 1, 5← 6, 0, 6	Ground							21 511.17	.2	358
		7, 1, 6← 7, 0, 7	Ground							22 511.60	.2	358
		8, 1, 7← 8, 0, 8	Ground							23 692.14	.2	358
		10, 1, 9←10, 0,10	Ground							26 645.25	.2	358
		11, 1,10←11, 0,11	Ground							28 445.64	.2	358
$C^{13}H_2Cl^{35}Si^{28}H_3$	233	4, 0, 4← 3, 0, 3	Ground							24 485.55	.05	324
		4, 1, 3← 3, 1, 2	Ground			7/2	9/2	5/2	7/2	25 068.4	.1	324
		4, 1, 3← 3, 1, 2	Ground							25 068.86	.2	358
		4, 1, 3← 3, 1, 2	Ground			5/2	11/2	3/2	9/2	25 069.3	.1	324
		4, 1, 4← 3, 1, 3	Ground			5/2	7/2	3/2	5/2	23 953.1	.1	324
		4, 1, 4← 3, 1, 3	Ground							23 953.63	.2	358
		4, 1, 4← 3, 1, 3	Ground			9/2	11/2	7/2	9/2	23 953.9	.1	324
		5, 0, 5← 4, 0, 4	Ground							30 582.3	.1	324
		5, 0, 5← 4, 0, 4	Ground							30 582.35	.2	358
		5, 1, 4← 4, 1, 3	Ground			9/2	11/2	7/2	9/2	31 329.88	.05	324
		5, 1, 4← 4, 1, 3	Ground							31 330.29	.2	358
		5, 1, 4← 4, 1, 3	Ground			7/2	13/2	5/2	11/2	31 330.68	.05	324
		5, 1, 5← 4, 1, 4	Ground			7/2	9/2	5/2	7/2	29 935.7	.1	324
		5, 1, 5← 4, 1, 4	Ground							29 936.02	.2	358
		5, 1, 5← 4, 1, 4	Ground			11/2	13/2	9/2	11/2	29 936.2	.1	324
		6, 0, 6← 5, 1, 5	Ground				9/2		7/2	20 643.52	.05	324
		6, 0, 6← 5, 1, 5	Ground				15/2		13/2	20 644.81	.05	324
		6, 0, 6← 5, 1, 5	Ground				11/2		9/2	20 646.97	.05	324
		6, 0, 6← 5, 1, 5	Ground				13/2		11/2	20 648.29	.05	324
		8, 1, 7← 8, 0, 8	Ground				13/2		13/2	23 542.4	.1	324
		8, 1, 7← 8, 0, 8	Ground				19/2		19/2	23 543.7	.1	324
		8, 1, 7← 8, 0, 8	Ground							23 546.17	.2	358
		8, 1, 7← 8, 0, 8	Ground				17/2		17/2	23 549.7	.1	324
		9, 1, 8← 9, 0, 9	Ground				15/2		15/2	25 077.48	.05	324
		9, 1, 8← 9, 0, 9	Ground				21/2		21/2	25 078.50	.05	324

1. See footnote preceding page.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_2Cl^{35}Si^{28}H_3$	233	9, 1, 8← 9, 0, 9	Ground						25 081.23	.2	358
		9, 1, 8← 9, 0, 9	Ground			17/2		17/2	25 083.90	.05	324
		9, 1, 8← 9, 0, 9	Ground			19/2		19/2	25 084.85	.05	324
		10, 1, 9←10, 0,10	Ground			17/2		17/2	26 848.5	.1	324
		10, 1, 9←10, 0,10	Ground			23/2		23/2	26 849.4	.1	324
		10, 1, 9←10, 0,10	Ground						26 852.29	.2	358
		10, 1, 9←10, 0,10	Ground			19/2		19/2	26 855.1	.1	324
		10, 1, 9←10, 0,10	Ground			21/2		21/2	26 856.0	.1	324
		11, 1,10←11, 0,11	Ground			19/2		19/2	28 870.45	.05	324
		11, 1,10←11, 0,11	Ground			25/2		25/2	28 871.18	.05	324
		11, 1,10←11, 0,11	Ground						28 874.24	.2	358
		11, 1,10←11, 0,11	Ground			21/2		21/2	28 877.25	.05	324
		11, 1,10←11, 0,11	Ground			23/2		23/2	28 877.90	.05	324
$C^{12}H_2Cl^{35}Si^{29}H_3$	234	4, 0, 4← 3, 0, 3	Ground						24 179.0	.1	324
		4, 0, 4← 3, 0, 3	Ground						24 179.60	.2	358
		4, 1, 3← 3, 1, 2	Ground		7/2	9/2	5/2	7/2	24 718.0	.1	324
		4, 1, 3← 3, 1, 2	Ground		5/2	11/2	3/2	9/2	24 718.0	.1	324
		4, 1, 3← 3, 1, 2	Ground						24 718.01	.2	358
		5, 0, 5← 4, 0, 4	Ground						30 203.92	.05	324
		5, 0, 5← 4, 0, 4	Ground						30 203.97	.2	358
		5, 1, 4← 4, 1, 3	Ground		7/2	13/2	5/2	11/2	30 892.78	.05	324
		5, 1, 4← 4, 1, 3	Ground		9/2	11/2	7/2	9/2	30 892.78	.05	324
		5, 1, 4← 4, 1, 3	Ground						30 892.79	.2	358
		5, 1, 5← 4, 1, 4	Ground		7/2	9/2	5/2	7/2	29 599.25	.05	324
		5, 1, 5← 4, 1, 4	Ground		11/2	13/2	9/2	11/2	29 599.25	.05	324
		5, 1, 5← 4, 1, 4	Ground						29 599.32	.2	358
		7, 0, 7← 6, 1, 6	Ground			11/2		9/2	26 075.08	.05	324
		7, 0, 7← 6, 1, 6	Ground			17/2		15/2	26 076.00	.05	324
		7, 0, 7← 6, 1, 6	Ground			13/2		11/2	26 078.28	.05	324
		7, 0, 7← 6, 1, 6	Ground			15/2		13/2	26 079.28	.05	324
		8, 1, 7← 8, 0, 8	Ground			19/2		19/2	23 776.2	.1	324
		8, 1, 7← 8, 0, 8	Ground						23 779.57	.2	358
		8, 1, 7← 8, 0, 8	Ground			17/2		17/2	23 782.8	.1	324
		9, 1, 8← 9, 0, 9	Ground			15/2		15/2	25 180.8	.1	324
		9, 1, 8← 9, 0, 9	Ground			21/2		21/2	25 181.6	.1	324
		9, 1, 8← 9, 0, 9	Ground						25 184.38	.2	358
		9, 1, 8← 9, 0, 9	Ground			17/2		17/2	25 187.0	.1	324
		9, 1, 8← 9, 0, 9	Ground			19/2		19/2	25 187.9	.1	324
		10, 1, 9←10, 0,10	Ground			17/2		17/2	26 790.7	.1	324
		10, 1, 9←10, 0,10	Ground			23/2		23/2	26 791.7	.1	324
		10, 1, 9←10, 0,10	Ground						26 794.74	.2	358
		10, 1, 9←10, 0,10	Ground			19/2		19/2	26 797.7	.1	324
		10, 1, 9←10, 0,10	Ground			21/2		21/2	26 798.7	.1	324
		11, 1,10←11, 0,11	Ground			25/2		25/2	28 626.79	.05	324
		11, 1,10←11, 0,11	Ground						28 630.20	.2	358
		11, 1,10←11, 0,11	Ground			23/2		23/2	28 633.52	.05	324
$C^{12}D_2Cl^{35}Si^{28}H_3$	235	4, 0, 4← 3, 0, 3	Ground	1					23 992.05	.2	358
		4, 0, 4← 3, 0, 3	Ground						24 095.95	.2	358
		4, 1, 3← 3, 1, 2	Ground	1					24 631.06	.2	358

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_2Cl^{35}Si^{28}H_3$	235	4, 1, 3← 3, 1, 2	Ground						24 752.39	.2	358
		4, 1, 4← 3, 1, 3	Ground	1					23 429.48	.2	358
		4, 1, 4← 3, 1, 3	Ground						23 519.83	.2	358
		5, 0, 5← 4, 0, 4	Ground	1					29 954.65	.2	358
		5, 1, 4← 4, 1, 3	Ground	1					30 779.07	.2	358
		5, 1, 4← 4, 1, 3	Ground						30 930.22	.2	358
		5, 1, 5← 4, 1, 4	Ground	1					29 277.72	.2	358
		5, 1, 5← 4, 1, 4	Ground						29 389.83	.2	358
		7, 1, 6← 7, 0, 7	Ground						19 057.54	.2	358
		8, 1, 7← 8, 0, 8	Ground	1					20 397.79	.2	358
		8, 1, 7← 8, 0, 8	Ground						20 593.01	.2	358
		9, 1, 8← 9, 0, 9	Ground						22 399.13	.2	358
		10, 1, 9←10, 0,10	Ground						24 495.28	.2	358
		12, 1,11←12, 0,12	Ground	1					29 142.97	.2	358
		12, 1,11←12, 0,12	Ground						29 613.69	.2	358
$C^{12}HDCl^{35}Si^{28}H_3$	236	4, 0, 4← 3, 0, 3	Ground						24 316.27	.2	358
		5, 1, 4← 4, 1, 3	Ground						31 156.99	.2	358
		5, 1, 5← 4, 1, 4	Ground						29 696.89	.2	358
		5, 1, 4← 5, 0, 5	Ground						18 508.34	.2	358
		6, 1, 5← 6, 0, 6	Ground						19 490.20	.2	358
		8, 1, 7← 8, 0, 8	Ground						22 089.27	.2	358
		9, 1, 8← 9, 0, 9	Ground						23 742.34	.2	358
$C^{12}H_2Cl^{35}Si^{28}D_3$	237	4, 0, 4← 3, 0, 3	Ground	1					22 435.80	.2	358
		4, 0, 4← 3, 0, 3	Ground						22 508.38	.2	358
		4, 1, 3← 3, 1, 2	Ground						22 964.29	.2	358
		4, 1, 4← 3, 1, 3	Ground						22 091.50	.2	358
		5, 0, 5← 4, 0, 4	Ground	1					28 028.14	.2	358
		5, 0, 5← 4, 0, 4	Ground						28 116.99	.2	358
		5, 1, 4← 4, 1, 3	Ground	1					28 592.69	.2	358
		5, 1, 4← 4, 1, 3	Ground						28 700.44	.2	358
		5, 1, 5← 4, 1, 4	Ground	1					27 534.57	.2	358
		5, 1, 5← 4, 1, 4	Ground						27 609.21	.2	358
		7, 1, 6← 7, 0, 7	Ground						18 011.15	.2	358
		8, 1, 7← 8, 0, 8	Ground						19 034.52	.2	358
		9, 1, 8← 9, 0, 9	Ground	1					20 003.13	.2	358
		9, 1, 8← 9, 0, 9	Ground						20 228.29	.2	358
		10, 1, 9←10, 0,10	Ground	1					21 330.46	.2	358
		10, 1, 9←10, 0,10	Ground						21 604.26	.2	358
		11, 1,10←11, 0,11	Ground	1					22 844.72	.2	358

CH_5FSi $C_s(C_{3v}.C_s)$ CH_3SiH_2F

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Si^{28}H_2F^{19}$	C_s	241	20 050. M	6 753.80 M	5 545.26 M				
$C^{12}H_3Si^{29}H_2F^{19}$	C_s	242	19 848. M	6 753.94 M	5 529.58 M				
$C^{12}H_3Si^{30}H_2F^{19}$	C_s	243	19 657. M	6 753.92 M	5 514.79 M				
$C^{12}D_3Si^{28}H_2F^{19}$	C_s	244	17 412. M	5 786.60 M	4 846.70 M				
$C^{12}H_3Si^{28}D_2F^{19}$	C_s	245	15 954. M	6 493.07 M	5 335.23 M				
$C^{12}D_3Si^{30}H_2F^{19}$	C_s	246	17 087. M	5 784.62 M	4 819.59 M				
s-$C^{12}H_2DSi^{28}H_2F^{19}$	C_s	247	20 000. M	6 270.63 M	5 212.80 M				
a-$C^{12}H_2DSi^{28}H_2F^{19}$	C_1	248	18 630. M	6 454.62 M	5 317.16 M				
$C^{13}H_3Si^{28}H_2F^{19}$	C_s	249	19 900. M	6 542.15 M	5 390.80 M				
$C^{12}D_3Si^{29}H_2F^{19}$	C_s	251	17 248. M	5 785.63 M	4 832.80 M				
$C^{12}H_3Si^{28}HDF^{19}$	C_s	252	17 855. M	6 636.34 M	5 427.57 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
241	1.67 M	0.39 M	0. X		1559	30					

References:

ABC: 233, 290

μ: 233

D_J:

eQq:

D_{JK}:

V: 233

κ:

I:

Δ:

ω:

Coupling parameter: $I_\alpha = 3.132$ amu Å^2. Ref: 233. Torsional frequency 261 cm^{-1}. Ref: 209.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Si^{28}H_2F^{19}$	241	2, 0, 2← 1, 0, 1	Ground	A	1					24 492.10	.10	233
		2, 0, 2← 1, 0, 1	Ground	E	1					24 500.10	.10	233
		2, 0, 2← 1, 0, 1	Ground							24 519.10	.10	233
		2, 1, 1← 1, 1, 0	Ground	E	1					25 630.50	.10	233
		2, 1, 1← 1, 1, 0	Ground	A	0					25 771.30	.10	233
		2, 1, 1← 1, 1, 0	Ground							25 806.77	.10	233
		2, 1, 2← 1, 1, 1	Ground	A	1					23 370.40	.10	233
		2, 1, 2← 1, 1, 1	Ground							23 389.50	.10	233
		2, 1, 2← 1, 1, 1	Ground	E	1					23 531.00	.10	233
		3, 0, 3← 2, 0, 2	Ground							36 583.44	.10	233
		3, 1, 2← 2, 1, 1	Ground	E	0					38 658.40	.10	151
		3, 1, 2← 2, 1, 1	Ground	A	0					38 658.92	.10	151
		3, 2, 1← 2, 2, 0	Ground							37 210.60	.10	233
		3, 2, 2← 2, 2, 1	Ground							36 897.80	.10	233
		5, 1, 4← 5, 1, 5	Ground	E	0					18 038.80	.10	233
		5, 1, 4← 5, 1, 5	Ground	A	0					18 040.50	.10	233
		6, 1, 5← 6, 1, 6	Ground	E	0					25 110.42	.10	233
		6, 1, 5← 6, 1, 6	Ground	A	0					25 113.08	.10	233
		7, 1, 6← 7, 1, 7	Ground	E	0					33 175.33	.10	233
		7, 1, 6← 7, 1, 7	Ground	A	0					33 178.93	.10	233
		9, 2, 7← 9, 2, 8	Ground	E	0					19 693.37	.10	233
		9, 2, 7← 9, 2, 8	Ground	A	0					19 694.15	.10	233
		10, 2, 8←10, 2, 9	Ground	E	0					27 060.92	.10	233
		10, 2, 8←10, 2, 9	Ground	A	0					27 062.30	.10	233
		Not Reported								17 571.94	.1	151
		Not Reported								17 573.95	.1	151
		Not Reported								20 035.0	.1	151
		Not Reported								20 263.58	.1	151
		Not Reported								21 923.25	.1	151
		Not Reported								21 924.75	.1	151
		Not Reported								23 383.04	.1	151
		Not Reported								25 492.96	.1	151
		Not Reported								25 771.34	.1	151
		Not Reported								26 402.76	.1	151
		Not Reported								26 405.2	.1	151
		Not Reported								26 519.40	.1	151
		Not Reported								26 589.80	.1	151
		Not Reported								26 741.37	.1	151
		Not Reported								26 745.20	.1	151
		Not Reported								28 695.25	.1	151
$C^{12}H_3Si^{29}H_2F^{19}$	242	2, 0, 2← 1, 0, 1	Ground							24 484.70	.10	233
		2, 1, 1← 1, 1, 0	Ground							25 791.38	.10	233
		2, 1, 2← 1, 1, 1	Ground							23 342.66	.10	233
$C^{12}H_3Si^{30}H_2F^{19}$	243	2, 0, 2← 1, 0, 1	Ground							24 451.59	.10	233
		2, 1, 1← 1, 1, 0	Ground							25 776.55	.10	233
		2, 1, 2← 1, 1, 1	Ground							23 298.30	.10	233
$C^{12}D_3Si^{28}H_2F^{19}$	244	2, 0, 2← 1, 0, 1	Ground		1					21 197.28	.10	290
		2, 0, 2← 1, 0, 1	Ground							21 211.54	.10	233
		2, 1, 1← 1, 1, 0	Ground		1					22 183.99	.10	290

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3Si^{28}H_2F^{19}$	244	2, 1, 1← 1, 1, 0	Ground							22 206.50	.10	233
		2, 1, 2← 1, 1, 1	Ground		1					20 319.39	.10	290
		2, 1, 2← 1, 1, 1	Ground							20 326.70	.10	233
		3, 0, 3← 2, 0, 2	Ground							31 681.20	.10	233
		3, 1, 2← 2, 1, 1	Ground							33 274.15	.10	233
		3, 2, 1← 2, 2, 0	Ground							32 117.38	.10	233
		6, 1, 5← 6, 1, 6	Ground							19 573.03	.10	233
		7, 1, 6← 7, 1, 7	Ground							25 908.00	.10	233
		10, 2, 8←10, 2, 9	Ground							19 793.05	.10	233
		11, 2, 9←11, 2,10	Ground							26 256.50	.10	233
$C^{12}H_3Si^{28}D_2F^{19}$	245	2, 0, 2← 1, 0, 1	Ground	A	1					23 530.00	.10	233
		2, 0, 2← 1, 0, 1	Ground	E	1					23 536.25	.10	233
		2, 0, 2← 1, 0, 1	Ground							23 556.56	.10	233
		2, 1, 1← 1, 1, 0	Ground							24 814.44	.10	233
		2, 1, 2← 1, 1, 1	Ground							22 498.71	.10	233
		3, 0, 3← 2, 0, 2	Ground							35 089.71	.10	233
		3, 2, 2← 2, 2, 1	Ground							35 485.60	.10	233
		5, 1, 4← 5, 1, 5	Ground	E	0					17 215.30	.10	233
		5, 1, 4← 5, 1, 5	Ground	A	0					17 216.80	.10	233
		6, 1, 5← 6, 1, 6	Ground	E	0					23 865.70	.10	233
		6, 1, 5← 6, 1, 6	Ground	A	0					23 868.02	.10	233
		8, 2, 6← 8, 2, 7								15 547.9	.1	151
		9, 2, 7← 9, 2, 8	Ground	E	0					21 019.80	.10	233
		9, 2, 7← 9, 2, 8	Ground	A	0					21 021.05	.10	233
		10, 2, 8←10, 2, 9	Ground	E	0					29 530.95	.10	233
		10, 2, 8←10, 2, 9	Ground	A	0					29 532.75	.10	233
$C^{12}D_3Si^{30}H_2F^{19}$	246	2, 0, 2← 1, 0, 1	Ground		1					21 134.95	.10	290
		2, 0, 2← 1, 0, 1	Ground							21 148.76	.10	290
		2, 1, 1← 1, 1, 0	Ground		1					22 151.	1.	290
		2, 1, 1← 1, 1, 0	Ground							22 173.46	.10	290
		2, 1, 2← 1, 1, 1	Ground		1					20 236.06	.10	290
		2, 1, 2← 1, 1, 1	Ground							20 243.40	.10	290
		3, 0, 3← 2, 0, 2	Ground							31 577.4	1.	290
		3, 1, 2← 2, 1, 1	Ground							33 224.40	.10	290
		3, 1, 3← 2, 1, 2	Ground							30 328.58	.10	290
		3, 2, 2← 2, 2, 1	Ground							31 813.56	.10	290
s-$C^{12}H_2DSi^{28}H_2F^{19}$	247	2, 0, 2← 1, 0, 1	Ground							22 907.78	.10	233
		2, 1, 1← 1, 1, 0	Ground							24 024.70	.10	233
		2, 1, 2← 1, 1, 1	Ground							21 909.03	.10	233
		2, 0, 3← 2, 0, 2	Ground							34 215.20	.10	233
		3, 1, 2← 2, 1, 1	Ground							35 999.00	.10	233
		3, 1, 3← 2, 1, 2	Ground							32 827.38	.10	233
		7, 1, 6← 7, 1, 7	Ground							29 194.80	.10	233
		10, 2, 8←10, 2, 9	Ground							21 694.80	.10	233
		11, 2, 9←11, 2,10	Ground							28 864.70	.10	233
a-$C^{12}H_2DSi^{28}H_2F^{19}$	248	2, 0, 2← 1, 0, 1	Ground							23 467.05	.1	233
		2, 1, 1← 1, 1, 0	Ground							24 681.03	.1	233
		2, 1, 2← 1, 1, 1	Ground							22 406.41	.1	233
		2, 0, 3← 2, 0, 2	Ground							35 013.50	.1	233

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
a-$C^{12}H_2DSi^{28}H_2F^{19}$	248	3, 1, 2← 2, 1, 1	Ground							36 972.82	.1	233
		3, 1, 3← 2, 1, 2	Ground							33 562.20	.1	233
		3, 2, 1← 2, 2, 0	Ground							35 616.20	.1	233
		3, 2, 2← 2, 2, 1	Ground							35 315.64	.1	233
		6, 1, 5← 6, 1, 6	Ground							23 626.60	.1	233
		7, 1, 6← 7, 1, 7	Ground							31 201.	1.	233
$C^{13}H_3Si^{28}H_2F^{19}$	249	2, 0, 2← 1, 0, 1	Ground							23 794.44	.10	233
		2, 1, 1← 1, 1, 0	Ground							25 017.26	.10	233
		2, 1, 2← 1, 1, 1	Ground							22 714.55	.10	233
		3, 0, 3← 2, 0, 2	Ground							35 514.66	.10	233
		3, 1, 2← 2, 1, 1	Ground							37 479.80	.10	233
		3, 2, 1← 2, 2, 0	Ground							36 083.60	.10	233
		3, 2, 2← 2, 2, 1	Ground							35 799.60	.10	233
		10, 2, 8←10, 2, 9	Ground	E	0					25 091.04	.10	233
		10, 2, 8←10, 2, 9	Ground	A	0					25 091.97	.10	233
		11, 2, 9←11, 2,10	Ground	E	0					33 106.55	.10	233
		11, 2, 9←11, 2,10	Ground	A	0					33 109.80	.10	233
$C^{12}D_3Si^{29}H_2F^{19}$	251	2, 0, 2← 1, 0, 1	Ground		1					21 165.26	.10	290
		2, 0, 2← 1, 0, 1	Ground							21 179.40	.10	290
		2, 1, 1← 1, 1, 0	Ground		1					22 167.26	.10	290
		2, 1, 1← 1, 1, 0	Ground							22 189.69	.10	290
		2, 1, 2← 1, 1, 1	Ground		1					20 276.44	.10	290
		2, 1, 2← 1, 1, 1	Ground							20 284.02	.10	290
		3, 0, 3← 2, 0, 2	Ground							31 628.73	.10	290
		3, 1, 3← 2, 1, 2	Ground							30 391.14	.10	290
		3, 2, 2← 2, 2, 1	Ground							31 854.5	.10	290
$C^{12}H_3Si^{28}HDF^{19}$	252	2, 0, 2← 1, 0, 1	Ground							24 034.80	.10	233
		2, 1, 1← 1, 1, 0	Ground							25 336.60	.10	233
		2, 1, 2← 1, 1, 1	Ground							22 919.05	.10	233
		3, 0, 3← 2, 0, 2	Ground							35 825.50	.10	233
		3, 1, 2← 2, 1, 1	Ground							37 943.80	.10	233
		3, 1, 3← 2, 1, 2	Ground							34 322.20	.10	233
		3, 2, 1← 2, 2, 0	Ground							36 192.50	.10	233

CH_5N $C_s(C_{3v},C_s)$ CH_3NH_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3N^{14}H_2$	C_s	261	22 626.1 M	21 703.1 M	10 314.8 M				
$C^{12}D_3N^{14}D_2$	C_s	262	52 401.00 M	16 549.52 M	15 571.72 M				199.66

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
261	0.304 M	0. X	1.247 M		1980						
262	0.265 M	0. X	1.299 M		684.7	2					

References:

ABC: 180, 187 D_J: D_{JK}: κ: Δ: 180

μ: 180 eQq: V: 180, 344 I: ω:

Add. Refs.: 22, 56, 74, 82, 83, 91, 96, 97, 117, 138, 168

For species 261, the quadrupole coupling constants are: $\chi_{aa}=2.3$ MHz, $\chi_{bb}=2.0$ MHz, $\chi_{cc}=-4.3$ MHz. Ref: 180. Its inversion splitting constant is 28604 MHz. Ref: 173. Its torsional frequency is 264 cm^{-1}. Ref: 168. $\Delta_0=29358$ MHz for N=1. Ref: 139. For species 262, the quadrupole coupling constants are: $\chi_{aa}=2.35$ MHz, $\chi_{bb}=2.12$ MHz, and $\chi_{cc}=-4.47$ MHz. Ref: 180. Its inversion splitting constant is 2246 ± 5 MHz. Ref: 173. Its torsional frequency is 201 cm^{-1}. Ref: 168.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	2, 0, ← 1, 1,	Ground							9 706.10	.1	379
		2, 0, ← 1, 1,	Ground							18 308.64		378
		4, 2, ← 5, 1,	Ground							10 262.41	.1	379
		4, 2, ← 5, 1,	Ground							14 437.67	.1	379
		4, 2, ← 5, 1,	Ground							17 475.66	.1	379
		4, 2, ← 5, 1,	Ground							17 476.28	.1	379
		4, 2, ← 5, 1,	Ground							19 776.01	.1	379
		4, 2, ← 5, 1,	Ground							19 777.85	.1	379
		4, 2, ← 5, 1,	Ground							23 340.67	.04	379
		4, 2, ← 5, 1,	Ground							23 341.31	.1	379[1]
		4, 2, ← 5, 1,	Ground							28 533.92	.1	379
		4, 2, ← 5, 1,	Ground	A	0					30 565.9		91
		4, 2, ← 5, 1,	Ground	A	0					36 452.1		91[1]
		4, 2, ← 5, 1,	Ground	E(−)	0					28 534.		187
		6, 1, ← 5, 2,	Ground							12 592.65	.1	379
		6, 1, ← 5, 2,	Ground							13 175.80		378
		6, 1, ← 5, 2,	Ground							13 177.34		378
		6, 1, ← 5, 2,	Ground							21 930.00	.1	379
		6, 1, ← 5, 2,	Ground							21 931.48	.1	379
		6, 1, ← 5, 2,	Ground							23 449.39	.1	379
		6, 1, ← 5, 2,	Ground							23 449.65	.1	379
		6, 1, ← 5, 2,	Ground							23 450.17	.1	379[1]
		6, 1, ← 5, 2,	Ground	A	0					29 312.4		91
		6, 1, ← 5, 2,	Ground	E(+)	0					29 771.4		91
		6, 1, ← 5, 2,	Ground	E(−)	0					13 176.		187
		6, 1, ← 6, 1,	Ground							18 475.8		378
		6, 1, ← 6, 1,	Ground							18 482.4		378
		7, 1, ← 7, 1,	Ground							24 634.04		378
		7, 1, ← 7, 1,	Ground							24 647.08		378
		7, 3, ← 8, 2,	Ground	A	0					46 545.		187
		7, 3, ← 8, 2,	Ground	A	0					48 082.		187
		7, 3, ← 8, 2,	Ground	A	0					48 387.		187
		7, 3, ← 8, 2,	Ground	A	0					49 915.		187
		8, 3, ← 9, 2,	Ground	E(−)	0					4 660.		187
		8, 3, ← 9, 2,	Ground	A	0					5 767.		187
		8, 3, ← 9, 2,	Ground	E(+)	0					6 450.		187
		8, 3, ← 9, 2,	Ground	E(−)	0					6 867.		187
		8, 3, ← 9, 2,	Ground							15 907.61	.1	379
		10, 2, ← 9, 3,	Ground							28 515.45	.1	379
		10, 2, ← 9, 3,	Ground							41 658.42		378
		10, 2, ← 9, 3,	Ground							43 498.32		378
		10, 2, ← 9, 3,	Ground							49 229.64		378
		10, 1, ←10, 1,	Ground							48 392.46		378
		10, 1, ←10, 1,	Ground							48 400.26		378
		11, 4, ←12, 3,	Ground							23 683.17	.1	379
		11, 4, ←12, 3,	Ground							23 861.40	.04	379
		11, 4, ←12, 3,	Ground	A	0					32 104.		187
		11, 4, ←12, 3,	Ground	A	0					32 283.		187
		11, 4, ←12, 3,	Ground	E(−)	0					32 708.		187
		11, 4, ←12, 3,	Ground	E(−)	0					43 040.72		378

1. Tentative assignments of the following lines were made by D. R. Lide, Jr. in a letter to the Journal of Chemical Physics *20*, 1812, (1952):

$4_{2,2} \leftarrow 5_{1,4}$	23,340.92 MHz.
$6_{1,5} \leftarrow 5_{2,3}$	23,449.90 MHz.
$4_{2,3} \leftarrow 5_{1,5}$	36,452.60 MHz.

However, in a later publication, these lines were not identified and have been so recorded.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	11, 4, ←12, 3,	Ground							43 404.8		378
		13, 3, ←12, 4,	Ground	E(+)	0					6 270.		187
		13, 3, ←12, 4,	Ground							8 411.94	.1	379
		13, 3, ←12, 4,	Ground							11 961.29	.1	379
		13, 3, ←12, 4,	Ground							12 162.44	.1	379
		13, 3, ←12, 4,	Ground	A	0					12 444.		187
		13, 3, ←12, 4,	Ground							20 547.17	.04	379
		13, 3, ←12, 4,	Ground							20 831.28	.04	379
		14, 3, ←13, 4,	Ground	E(−)	0					45 995.		187
		15, 5, ←16, 4,	Ground							12 238.84	.1	379
		15, 5, ←16, 4,	Ground							12 258.96	.1	379
		15, 5, ←16, 4,	Ground							16 681.80	.1	379
		15, 5, ←16, 4,	Ground							21 712.65	.1	379
		15, 5, ←16, 4,	Ground							23 409.16	.1	379
		15, 5, ←16, 4,	Ground							23 429.42	.1	379
		15, 5, ←16, 4,	Ground	E(−)	0					27 504.		187
		15, 5, ←16, 4,	Ground							27 758.40	.1	379
		17, 4, ←16, 5,	Ground							16 947.65	.1	379
		17, 4, ←16, 5,	Ground							21 019.17	.1	379
		17, 4, ←16, 5,	Ground							21 051.62	.1	379
		17, 4, ←16, 5,	Ground							22 722.62	.04	379
		17, 4, ←16, 5,	Ground	E(−)	0					22 723.		187
		17, 4, ←16, 5,	Ground	A	0					32 155.		187
		17, 4, ←16, 5,	Ground	A	0					32 187.		187
		17, 4, ←16, 5,	Ground	E(+)	0					33 152.		187
		18, 6, ←19, 5,	Ground	E(−)	0					45 958.		187
		18, 6, ←19, 5,	Ground	E(−)	0					47 335.		187
		18, 6, ←19, 5,	Ground	E(+)	0					48 415.		187
		18, 6, ←19, 5,	Ground	A	0					49 426.		187
		19, 6, ←20, 5,	Ground	A	0					4 858.		187
		19, 6, ←20, 5,	Ground	A	0					4 860.		187
		19, 6, ←20, 5,	Ground	E(+)	0					6 500.		187
		19, 6, ←20, 5,	Ground							13 415.33	.1	379
		19, 6, ←20, 5,	Ground							13 416.57	.1	379
		21, 5, ←20, 6,	Ground	A	0					30 565.		187
		21, 5, ←20, 6,	Ground	A	0					30 566.		187
		21, 5, ←20, 6,	Ground							42 104.30		378
		21, 5, ←20, 6,	Ground							42 804.58		378
		21, 5, ←20, 6,	Ground							43 346.58		378
		Not Reported								2 781.95	.5	138
		Not Reported								2 782.62	.5	138
		Not Reported								3 015.17	.5	138
		Not Reported								3 019.90	.5	138
		Not Reported								3 389.74	.5	138
		Not Reported								3 483.67	.5	138
		Not Reported								3 505.76	.5	138
		Not Reported								3 797.95	.5	138
		Not Reported								3 921.96	.5	138
		Not Reported								4 076.65	.01	138
		Not Reported								4 129.01	.5	138

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported							4 129.84	.5	138
		Not Reported							4 142.15	.5	138
		Not Reported							4 480.55	.5	138
		Not Reported							4 543.00	.5	138
		Not Reported							4 660.42	.5	138
		Not Reported							4 857.86	.5	138
		Not Reported							4 859.88	.5	138
		Not Reported							4 963.00	.5	138
		Not Reported							5 006.82	.5	138
		Not Reported							5 284.82	.01	138
		Not Reported							5 546.75	.5	138
		Not Reported							5 602.57	.5	138
		Not Reported							5 679.92	.5	138
		Not Reported							5 680.84	.5	138
		Not Reported							5 766.68	.5	138
		Not Reported							5 876.61	.5	138
		Not Reported							6 153.64	.5	138
		Not Reported							6 172.20	.5	138
		Not Reported							6 246.42	.5	138
		Not Reported							6 269.81	.5	138
		Not Reported							6 349.51	.5	138
		Not Reported							6 350.09	.5	138
		Not Reported							6 450.42	.5	138
		Not Reported							6 469.43	.5	138
		Not Reported							6 487.99	.5	138
		Not Reported							6 500.42	.5	138
		Not Reported							6 655.04	.01	138
		Not Reported							6 748.80	.5	138
		Not Reported							6 837.58	.5	138
		Not Reported							6 867.17	.5	138
		Not Reported	Ground						6 894.81	.04	97
		Not Reported	Ground						6 939.82	.1	97
		Not Reported	Ground						7 000.71	.1	97
		Not Reported	Ground						7 115.14	.1	97
		Not Reported	Ground						7 213.43	.1	97
		Not Reported	Ground						7 253.64	.1	97
		Not Reported							7 382.93	.01	138
		Not Reported							7 383.78	.01	138
		Not Reported							7 515.56	.5	138
		Not Reported	Ground						7 718.11	.1	97
		Not Reported	Ground						7 727.74	.04	97
		Not Reported	Ground						7 757.18	.1	97
		Not Reported	Ground						7 896.89	.1	97
		Not Reported	Ground						7 911.49	.04	97
		Not Reported	Ground						8 131.59	.1	97
		Not Reported	Ground						8 201.65	.04	97
		Not Reported	Ground						8 233.22	.1	97
		Not Reported	Ground						8 268.99	.1	97
		Not Reported	Ground						8 684.29	.04	97
		Not Reported	Ground						8 813.22	.1	97

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported	Ground						8 884.29	.1	97
		Not Reported	Ground						8 950.90	.1	97
		Not Reported	Ground						9 057.85	.04	97
		Not Reported	Ground						9 079.39	.04	97
		Not Reported	Ground						9 127.61	.04	97
		Not Reported	Ground						9 128.14	.04	97
		Not Reported	Ground						9 223.83	.1	97
		Not Reported	Ground						9 285.77	.1	97
		Not Reported	Ground						9 452.63	.1	97
		Not Reported	Ground						9 453.06	.1	97
		Not Reported	Ground						9 459.96	.1	97
		Not Reported	Ground						9 584.09	.1	97
		Not Reported	Ground						9 779.33	.04	97
		Not Reported	Ground						9 938.95	.04	97
		Not Reported	Ground						10 108.45	.1	97
		Not Reported	Ground						10 109.61	.1	97
		Not Reported	Ground						10 178.86	.1	97
		Not Reported	Ground						10 240.48	.04	97
		Not Reported	Ground						10 379.79	.1	97
		Not Reported	Ground						10 381.21	.1	97
		Not Reported	Ground						11 786.82		378
		Not Reported	Ground						11 819.80		378
		Not Reported	Ground						11 878.90	.04	97
		Not Reported	Ground						12 061.92	.1	97
		Not Reported	Ground						12 271.51	.1	97
		Not Reported	Ground						12 306.86	.1	97
		Not Reported	Ground						12 444.04	.04	97
		Not Reported	Ground						12 445.		378
		Not Reported	Ground						12 482.96	.04	97
		Not Reported	Ground						12 484.56	.04	97
		Not Reported	Ground						12 744.25	.04	97
		Not Reported	Ground						12 841.24	.1	97
		Not Reported	Ground						12 903.16	.1	97
		Not Reported	Ground						13 050.32	.1	97
		Not Reported	Ground						13 242.99	.1	97
		Not Reported	Ground						13 336.58	.1	97
		Not Reported	Ground						13 390.07	.1	97
		Not Reported	Ground						13 464.76	.1	97
		Not Reported	Ground						13 528.26	.04	97
		Not Reported	Ground						13 592.68	.1	97
		Not Reported	Ground						13 799.79	.1	97
		Not Reported	Ground						13 897.60	.1	97
		Not Reported	Ground						13 932.46	.04	97
		Not Reported	Ground						14 033.54	.04	97
		Not Reported	Ground						14 044.39	.04	97
		Not Reported	Ground						14 098.16	.1	97
		Not Reported	Ground						14 115.35	.1	97
		Not Reported	Ground						14 215.99	.1	97
		Not Reported	Ground						14 339.06	.1	97
		Not Reported	Ground						14 494.64	.04	97

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported	Ground						14 771.22	.1	97
		Not Reported	Ground						14 910.71	.04	97
		Not Reported	Ground						14 961.12		378
		Not Reported	Ground						15 047.43	.1	97
		Not Reported	Ground						15 094.56	.1	97
		Not Reported	Ground						15 109.45	.1	97
		Not Reported	Ground						15 141.72	.1	97
		Not Reported	Ground						15 146.16	.04	97
		Not Reported	Ground						15 252.52	.1	97
		Not Reported	Ground						15 357.69	.04	97
		Not Reported	Ground						15 397.72	.04	97
		Not Reported	Ground						15 842.14	.04	97
		Not Reported	Ground						15 999.68	.1	97
		Not Reported	Ground						16 088.98	.04	97
		Not Reported	Ground						16 089.84	.04	97
		Not Reported	Ground						16 228.00		378
		Not Reported	Ground						16 240.64	.1	97
		Not Reported	Ground						16 373.56		378
		Not Reported	Ground						16 410.63	.04	97
		Not Reported	Ground						16 661.73	.04	97
		Not Reported	Ground						16 670.02	.04	97
		Not Reported	Ground						16 742.98	.04	97
		Not Reported	Ground						16 911.46	.1	97
		Not Reported	Ground						17 042.46	.04	97
		Not Reported	Ground						17 108.99	.04	97
		Not Reported	Ground						17 148.36		378
		Not Reported	Ground						17 200.97	.04	97
		Not Reported	Ground						17 228.32	.1	97
		Not Reported	Ground						17 237.77	.1	97
		Not Reported	Ground						17 238.04	.1	97
		Not Reported	Ground						17 263.86	.1	97
		Not Reported	Ground						17 302.03	.04	97
		Not Reported	Ground						17 345.10	.1	97
		Not Reported	Ground						17 345.70	.1	97
		Not Reported	Ground						17 360.58	.1	97
		Not Reported	Ground						17 361.10	.1	97
		Not Reported	Ground						17 585.33	.1	97
		Not Reported	Ground						17 660.45	.1	97
		Not Reported	Ground						17 849.46	.04	97
		Not Reported	Ground						17 874.52	.1	97
		Not Reported	Ground						17 887.20	.1	97
		Not Reported	Ground						17 913.74	.04	97
		Not Reported	Ground						18 023.18	.1	97
		Not Reported	Ground						18 348.40		378
		Not Reported							18 486.		187
		Not Reported	Ground						18 562.40	.1	97
		Not Reported	Ground						18 680.50	.1	97
		Not Reported	Ground						18 884.52	.1	97
		Not Reported	Ground						18 928.16		378
		Not Reported	Ground						19 013.55	.04	97

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported	Ground						19 110.66	.04	97
		Not Reported	Ground						19 724.62	.04	97
		Not Reported	Ground						19 919.56	.04	97
		Not Reported	Ground						19 933.82	.1	97
		Not Reported	Ground						20 076.00	.04	97
		Not Reported	Ground						20 243.54	.04	97
		Not Reported	Ground						20 302.80		378
		Not Reported	Ground						20 325.82	.1	97
		Not Reported	Ground						20 911.74	.1	97
		Not Reported	Ground						20 947.05	.1	97
		Not Reported	Ground						20 971.70	.1	97
		Not Reported	Ground						20 973.15	.1	97
		Not Reported	Ground						21 013.62	.1	97
		Not Reported	Ground						21 027.06	.1	97
		Not Reported	Ground						21 035.13	.1	97
		Not Reported	Ground						21 244.56	.1	97
		Not Reported	Ground						21 297.12	.04	97
		Not Reported	Ground						21 477.62	.1	97
		Not Reported	Ground						21 614.33	.1	97
		Not Reported	Ground						21 765.23	.1	97
		Not Reported	Ground						21 842.31	.04	97
		Not Reported	Ground						22 060.71		378
		Not Reported	Ground						22 082.37		378
		Not Reported	Ground						22 112.46	.1	97
		Not Reported	Ground						22 258.35	.04	97
		Not Reported	Ground						22 369.95		378
		Not Reported	Ground						22 381.96		378
		Not Reported	Ground						22 507.42		378
		Not Reported	Ground						22 527.93	.04	97
		Not Reported	Ground						22 528.21	.04	97
		Not Reported	Ground						22 581.49	.1	97
		Not Reported	Ground						22 588.42	.1	97
		Not Reported	Ground						22 637.08		378
		Not Reported	Ground						22 759.22	.04	97
		Not Reported	Ground						22 759.63	.1	97
		Not Reported	Ground						22 765.62	.1	97
		Not Reported	Ground						22 818.83		378
		Not Reported	Ground						22 980.95	.1	97
		Not Reported	Ground						22 981.60	.1	97
		Not Reported	Ground						23 071.58		378
		Not Reported	Ground						23 090.83		378
		Not Reported	Ground						23 106.34		378
		Not Reported	Ground						23 119.06	.04	97
		Not Reported	Ground						23 219.21	.1	97
		Not Reported	Ground						23 300.79	.1	97
		Not Reported	Ground						23 311.31	.1	97
		Not Reported	Ground						23 315.55	.1	97
		Not Reported	Ground						23 424.70	.1	97
		Not Reported	Ground						23 432.84	.1	97
		Not Reported	Ground						23 608.52		378

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported	Ground						23 873.61	.04	97
		Not Reported	Ground						24 019.01	.1	97
		Not Reported	Ground						24 037.31		378
		Not Reported	Ground						24 078.75	.1	97
		Not Reported	Ground						24 320.57	.1	97
		Not Reported	Ground						24 382.16	.1	97
		Not Reported	Ground						24 465.58		378
		Not Reported	Ground						24 472.77		378
		Not Reported	Ground						24 520.75	.1	97
		Not Reported	Ground						24 889.42	.04	97
		Not Reported	Ground						24 889.80	.1	97
		Not Reported	Ground						24 993.76	.1	97
		Not Reported	Ground						25 063.65	.04	97
		Not Reported	Ground						25 206.62	.04	97
		Not Reported	Ground						25 401.99	.1	97
		Not Reported	Ground						25 507.61	.1	97
		Not Reported	Ground						25 810.49	.1	97
		Not Reported	Ground						25 810.96	.1	97
		Not Reported	Ground						25 861.23	.1	97
		Not Reported	Ground						26 134.72	.1	97
		Not Reported	Ground						26 339.57	.1	97
		Not Reported	Ground						26 448.15	.1	97
		Not Reported	Ground						26 487.00	.1	97
		Not Reported	Ground						26 493.54	.1	97
		Not Reported	Ground						26 493.82	.1	97
		Not Reported	Ground						26 588.65	.1	97
		Not Reported	Ground						26 654.86	.1	97
		Not Reported	Ground						26 695.43	.1	97
		Not Reported	Ground						26 717.89	.1	97
		Not Reported	Ground						26 728.77	.1	97
		Not Reported	Ground						26 733.54	.1	97
		Not Reported	Ground						27 323.13	.1	97
		Not Reported	Ground						27 445.47	.1	97
		Not Reported	Ground						27 504.75	.1	97
		Not Reported	Ground						27 553.24		378
		Not Reported	Ground						28 107.75	.04	97
		Not Reported	Ground						28 142.85	.04	97
		Not Reported	Ground						28 183.46	.1	97
		Not Reported	Ground						28 186.02	.1	97
		Not Reported	Ground						28 380.93	.1	97
		Not Reported	Ground						29 055.20	.1	97
		Not Reported	Ground						29 138.85	.1	97
		Not Reported	Ground						29 147.37	.1	97
		Not Reported	Ground						29 191.47	.1	97
		Not Reported	Ground						29 244.20	.1	97
		Not Reported	Ground						29 770.2		111
		Not Reported	Ground						29 771.40		111
		Not Reported	Ground						30 025.9		111
		Not Reported	Ground						30 088.5		111
		Not Reported	Ground						30 226.8		111

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported	Ground						30 236.7		111
		Not Reported	Ground						30 564.89		111
		Not Reported	Ground						30 566.42		111
		Not Reported	Ground						30 721.3		111
		Not Reported	Ground						31 140.5		111
		Not Reported	Ground						31 220.80		111
		Not Reported	Ground						31 221.20		111
		Not Reported	Ground						31 328.0		111
		Not Reported	Ground						31 583.41		111
		Not Reported	Ground						31 583.87		111
		Not Reported	Ground						31 846.1		111
		Not Reported	Ground						32 104.0		111
		Not Reported	Ground						32 112.7		111
		Not Reported	Ground						32 155.3		111
		Not Reported	Ground						32 187.0		111
		Not Reported	Ground						32 279.9		111
		Not Reported	Ground						32 283.3		111
		Not Reported	Ground						32 287.7		111
		Not Reported	Ground						32 634.2		111
		Not Reported	Ground						32 709.0		111
		Not Reported	Ground						32 916.8		111
		Not Reported	Ground						32 985.3		111
		Not Reported	Ground						33 136.5		111
		Not Reported	Ground						33 152.3		111
		Not Reported	Ground						33 302.0		111
		Not Reported	Ground						33 386.4		111
		Not Reported	Ground						33 388.2		111
		Not Reported	Ground						33 422.3		111
		Not Reported	Ground						33 506.8		111
		Not Reported	Ground						33 563.3		111
		Not Reported	Ground						33 599.1		111
		Not Reported	Ground						33 619.9		111
		Not Reported	Ground						33 631.5		111
		Not Reported	Ground						33 636.8		111
		Not Reported	Ground						33 639.5		111
		Not Reported	Ground						33 654.3		111
		Not Reported	Ground						33 862.2		111
		Not Reported	Ground						33 917.5		111
		Not Reported	Ground						33 990.5		111
		Not Reported	Ground						34 203.		111
		Not Reported	Ground						34 280.0		111
		Not Reported	Ground						34 314.3		111
		Not Reported	Ground						34 527.7		111
		Not Reported	Ground						34 623.8		111
		Not Reported	Ground						34 773.1		111
		Not Reported	Ground						34 835.1		111
		Not Reported	Ground						34 896.7		111
		Not Reported	Ground						34 907.8		111
		Not Reported	Ground						35 185.		111
		Not Reported	Ground						35 241.		111

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported	Ground						36 015.0		111
		Not Reported	Ground						36 452.1		111
		Not Reported	Ground						36 885.4		111
		Not Reported	Ground						36 957.5		111
		Not Reported	Ground						37 564.		111
		Not Reported	Ground						37 854.		111
		Not Reported	Ground						38 003.6		111
		Not Reported	Ground						41 615.12		187
		Not Reported	Ground						41 615.76		187
		Not Reported	Ground						41 658.42		378
		Not Reported	Ground						41 830.54		187
		Not Reported	Ground						42 101.94		187
		Not Reported	Ground						42 622.36		187
		Not Reported	Ground						42 720.94		187
		Not Reported	Ground						43 040.72		378
		Not Reported	Ground						43 220.12		187
		Not Reported	Ground						43 711.80		187
		Not Reported	Ground						43 728.61		187
		Not Reported	Ground						44 188.60		187
		Not Reported							44 205.		187
		Not Reported							44 214.		187
		Not Reported	Ground						44 286.76		187
		Not Reported	Ground						44 462.1		187
		Not Reported	Ground						44 573.06		187
		Not Reported	Ground						44 826.66		187
		Not Reported	Ground						44 967.40		187
		Not Reported	Ground						45 256.68		187
		Not Reported	Ground						45 324.22		187
		Not Reported	Ground						45 325.04		187
		Not Reported	Ground						45 336.60		187
		Not Reported	Ground						45 458.06		187
		Not Reported	Ground						45 759.26		187
		Not Reported	Ground						45 769.96		187
		Not Reported	Ground						45 865.08		187
		Not Reported	Ground						45 957.66		187
		Not Reported	Ground						45 994.56		187
		Not Reported	Ground						46 163.84		187
		Not Reported	Ground						46 368.42		187
		Not Reported	Ground						46 544.84		187
		Not Reported	Ground						46 575.18		187
		Not Reported	Ground						46 771.70		187
		Not Reported	Ground						46 855.6		187
		Not Reported	Ground						47 032.08		187
		Not Reported	Ground						47 075.84		187
		Not Reported	Ground						47 239.84		187
		Not Reported	Ground						47 334.60		187
		Not Reported	Ground						47 608.08		187
		Not Reported	Ground						47 732.44		187
		Not Reported	Ground						48 180.38		187
		Not Reported	Ground						48 243.46		187

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}H_2$	261	Not Reported								48 385.		187
		Not Reported	Ground							48 386.64		378
		Not Reported	Ground							48 404.06		187
		Not Reported	Ground							48 414.83		187
		Not Reported	Ground							48 547.14		187
		Not Reported	Ground							48 715.82		187
		Not Reported	Ground							48 857.40		187
		Not Reported	Ground							49 085.76		187
		Not Reported	Ground							49 086.38		187
		Not Reported	Ground							49 148.90		187
		Not Reported	Ground							49 426.06		187
		Not Reported	Ground							49 560.00		187
		Not Reported	Ground							49 614.02		187
		Not Reported	Ground							49 874.58		378
		Not Reported	Ground							49 952.46		187
		Not Reported	Ground							50 399.24		187
		Not Reported	Ground							50 423.40		187
		Not Reported	Ground							50 558.60		187
		Not Reported	Ground							50 658.48		187
		Not Reported	Ground							50 875.60		187
		Not Reported	Ground							50 934.64		187
		Not Reported	Ground							51 048.46		187
$C^{12}D_3N^{14}D_2$	262	1, 0, 1← 0, 0, 0	Ground							32 121.23		180
		1, 1, 1← 1, 0, 1	Ground	E	0					35 696.21		180
		1, 1, 1← 1, 0, 1	Ground	A	0					35 812.36		180
		1, 1, 1← 1, 0, 1	Ground	E	0					35 866.30		180
		1, 1, 1← 1, 0, 1	Ground	A	0					36 109.50		180
		2, 1, 2← 2, 0, 2	Ground	E	0					34 755.67		180
		2, 1, 2← 2, 0, 2	Ground	A	0					34 854.43		180
		2, 1, 2← 2, 0, 2	Ground	E	0					34 911.62		180
		2, 1, 2← 2, 0, 2	Ground	A	0					35 151.58		180
		3, 1, 3← 3, 0, 3	Ground	E	0					33 360.49		180
		3, 1, 3← 3, 0, 3	Ground	A	0					33 454.41		180
		3, 1, 3← 3, 0, 3	Ground	E	0					33 512.83		180
		3, 1, 3← 3, 0, 3	Ground	A	0					33 751.65		180
		4, 1, 3← 3, 2, 1	Ground	A	0					23 967.46		180
		4, 1, 3← 3, 2, 1	Ground	A	0					24 125.48		180
		4, 1, 3← 3, 2, 1	Ground	E	0					24 230.29		180
		4, 1, 3← 3, 2, 1	Ground	E	0					24 236.48		180
		4, 1, 3← 3, 2, 2	Ground	E	0					24 342.40		180
		4, 1, 3← 3, 2, 2	Ground	E	0					24 489.58		180
		4, 1, 4← 4, 0, 4	Ground	E	0					31 565.45		180
		4, 1, 4← 4, 0, 4	Ground	A	0					31 656.92		180
		4, 1, 4← 4, 0, 4	Ground	E	0					31 716.25		180
		4, 1, 4← 4, 0, 4	Ground	A	0					31 954.11		180
		5, 1, 5← 5, 0, 5	Ground	E	0					29 431.36		180
		5, 1, 5← 5, 0, 5	Ground	A	0					29 520.90		180
		5, 1, 5← 5, 0, 5	Ground	E	0					29 581.31		180
		5, 1, 5← 5, 0, 5	Ground	A	0					29 817.76		180

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3N^{14}D_2$	262	7, 1, 7← 7, 0, 7	Ground	E	0					24 446.85		180
		7, 1, 7← 7, 0, 7	Ground	A	0					24 531.04		180
		7, 1, 7← 7, 0, 7	Ground	E	0					24 595.38		180
		7, 1, 7← 7, 0, 7	Ground	A	0					24 826.54		180
$C^{12}D_3N^{14}H_2$	263	1, 0, 1← 0, 0, 0								36 436.2	.5	312
		1, 0, 1← 0, 0, 0								36 436.8	.5	312
		2, , ← 2, ,								28 601.6	.5	312
		3, , ← 2, ,								25 570.4	.5	312
		3, , ← 2, ,								27 815.0	.5	312
		3, , ← 3, ,								37 015.4	.5	312
		3, , ← 3, ,								37 951.4	.5	312
		4, , ← 3, ,								24 913.1	.5	312
		4, , ← 3, ,								31 656.2	.5	312
		4, , ← 4, ,								36 451.1	.5	312
		4, , ← 4, ,								37 386.3	.5	312
		5, , ← 5, ,								35 588.1	.5	312
		5, , ← 5, ,								35 590.6	.5	312
		6, , ← 6, ,								35 171.4	.5	312
		6, , ← 6, ,								37 427.1	.5	312
		7, , ← 6, ,								34 670.		312
		Not Reported								25 834.5	.5	312
		Not Reported								27 472.5	.5	312
		Not Reported								29 507.2	.5	312
		Not Reported								29 913.2	.5	312
		Not Reported								30 010.5	.5	312
		Not Reported								30 057.2	.5	312
		Not Reported								31 422.9	.5	312
		Not Reported								31 933.7	.5	312
		Not Reported								32 178.0	.5	312
		Not Reported								32 267.4	.5	312
		Not Reported								32 298.0	.5	312
		Not Reported								32 968.3	.5	312
		Not Reported								33 160.4	.5	312
		Not Reported								33 664.2	.5	312
		Not Reported								33 692.1	.5	312
		Not Reported								33 860.		312
		Not Reported								33 900.		312
		Not Reported								34 625.		312
		Not Reported								34 962.4	.5	312
		Not Reported								34 995.0	.5	312
		Not Reported								35 100.		312
		Not Reported								35 135.7	.5	312
		Not Reported								35 202.1	.5	312
		Not Reported								35 324.7	.5	312
		Not Reported								36 753.7	.5	312
		Not Reported								36 816.6	.5	312
		Not Reported								36 856.9	.5	312
		Not Reported								37 148.	10.	312
		Not Reported								37 230.	10.	312
		Not Reported								37 320.9	.5	312
		Not Reported								37 807.9	.5	312
		Not Reported								37 812.2	.5	312
		Not Reported								37 840.5	.5	312
		Not Reported								38 023.7	.5	312

CH_5P $C_s(C_{3v},C_s)$ CH_3PH_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3P^{31}H_2$	C_s	271	71 869.5 M	11 792.6 M	11 677.7 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
271	0.958 M	0. X	0.541 M		685.2	5					

References:

ABC: 325 D_J: D_{JK}: κ: Δ:

μ: 325 eQq: V: 325 I: ω:

Coupling parameter: $I_\alpha = 3.212$ amu Å^2. Ref: 325.

Methylphosphine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3P^{31}H_2$	271	1, 0, 1← 0, 0, 0	Ground	A	4					23 224.6	.1	325
		1, 0, 1← 0, 0, 0	Ground	E	3					23 250.0	.1	325
		1, 0, 1← 0, 0, 0	Ground	A	3					23 279.0	.1	325
		1, 0, 1← 0, 0, 0	Ground	A	2					23 314.8	.1	325
		1, 0, 1← 0, 0, 0	Ground	E	2					23 324.2	.1	325
		1, 0, 1← 0, 0, 0	Ground	E	1					23 394.8	.1	325
		1, 0, 1← 0, 0, 0	Ground	A	1					23 395.9	.1	325
		1, 0, 1← 0, 0, 0	Ground		0					23 470.3	.1	325
		1, 1, 0← 2, 0, 2	Ground	E	0					13 437.1	.1	325
		1, 1, 0← 2, 0, 2	Ground	A	0					13 451.8	.1	325
		1, 1, 1← 2, 0, 2	Ground	E	0					12 756.4	.1	325
		2, 0, 2← 1, 0, 1	Ground	E	1					46 789.2	.1	325
		2, 0, 2← 1, 0, 1	Ground	A	1					46 791.4	.1	325
		2, 0, 2← 1, 0, 1	Ground		0					46 940.1	.1	325
		2, 1, 1← 1, 1, 0	Ground	E	1					46 791.5	.1	325
		2, 1, 1← 1, 1, 0	Ground	A	1					46 895.1	.5	325
		2, 1, 1← 1, 1, 0	Ground	E	0					46 975.7	.1	325
		2, 1, 1← 1, 1, 0	Ground	A	0					47 052.2	.1	325
		2, 1, 2← 1, 1, 0	Ground	A	1					46 685.8	.1	325
		2, 1, 2← 1, 1, 1	Ground	E	1					46 787.4	.1	325
		2, 1, 2← 1, 1, 1	Ground	A	0					46 827.3	.1	325
		2, 1, 2← 1, 1, 1	Ground	E	0					46 904.6	.1	325
		4, 0, 4← 3, 1, 2	Ground	A	0					33 202.0	.1	325
		6, 2, 4← 7, 1, 6	Ground	E	0					14 695.6	.1	325
		6, 2, 4← 7, 1, 6	Ground	A	0					14 991.7	.1	325
		6, 2, 5← 7, 1, 7	Ground	E	0					17 142.2	.1	325
		6, 2, 5← 7, 1, 7	Ground	A	0					18 141.1	.1	325
		9, 1, 8← 8, 2, 6	Ground	A	0					32 864.5	.1	325
		9, 1, 8← 8, 2, 6	Ground	E	0					33 158.1	.1	325
		9, 1, 9← 8, 2, 7	Ground	A	0					27 819.0	.1	325
		9, 1, 9← 8, 2, 7	Ground	E	0					28 820.8	.1	325
		14, 2,12←13, 3,10	Ground	A	0					27 720.4	.1	325
		14, 2,12←13, 3,10	Ground	E	0					28 332.3	.1	325
		14, 2,13←13, 3,11	Ground	A	0					27 435.8	.1	325
		14, 2,13←13, 3,11	Ground	E	0					27 737.9	.1	325

CH_6Ge $C_{3v}(C_{3v},C_{3v})$ CH_3GeH_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Ge^{70}H_3$	C_{3v}	281		8 710.65 M	8 710.65 M		.025		
$C^{12}H_3Ge^{72}H_3$	C_{3v}	282		8 679.39 M	8 679.39 M				
$C^{12}H_3Ge^{73}H_3$	C_{3v}	283		8 664.44 M	8 664.44 M		.025		
$C^{12}H_3Ge^{74}H_3$	C_{3v}	284		8 649.68 M	8 649.68 M				
$C^{12}H_3Ge^{76}H_3$	C_{3v}	285		8 621.48 M	8 621.48 M				
$C^{13}H_3Ge^{70}H_3$	C_{3v}	286		8 337.34 M	8 337.34 M				
$C^{13}H_3Ge^{72}H_3$	C_{3v}	287		8 305.40 M	8 305.40 M				
$C^{13}H_3Ge^{74}H_3$	C_{3v}	288		8 275.09 M	8 275.09 M				
$C^{13}H_3Ge^{76}H_3$	C_{3v}	289		8 246.20 M	8 246.20 M				
$C^{12}H_3Ge^{70}D_3$	C_{3v}	291		7 993.00 M	7 993.00 M				
$C^{12}H_3Ge^{72}D_3$	C_{3v}	292		7 971.06 M	7 971.06 M				
$C^{12}H_3Ge^{74}D_3$	C_{3v}	293		7 950.08 M	7 950.08 M				
$C^{12}D_3Ge^{70}H_3$	C_{3v}	294		7 097.27 M	7 097.27 M				
$C^{12}D_3Ge^{72}H_3$	C_{3v}	295		7 067.29 M	7 067.29 M				
$C^{12}D_3Ge^{74}H_3$	C_{3v}	296		7 038.80 M	7 038.80 M				
$C^{12}H_3Ge^{70}H_2D$	C_s	297		8 600.70 M	8 313.68 M				
$C^{12}H_3Ge^{72}H_2D$	C_s	298		8 572.10 M	8 286.83 M				
$C^{12}H_3Ge^{74}H_2D$	C_s	299		8 544.89 M	8 261.25 M				
$C^{12}H_3Ge^{70}HD_2$	C_s	301		8 361.24 M	8 076.18 M				
$C^{12}H_3Ge^{72}HD_2$	C_s	302		8 335.64 M	8 052.44 M				
$C^{12}H_3Ge^{74}HD_2$	C_s	303		8 311.26 M	8 029.80 M				
$C^{12}H_2DGe^{70}H_3$	C_s	304		8 143.64 M	8 020.12 M				
$C^{12}H_2DGe^{72}H_3$	C_s	305		8 112.37 M	7 989.86 M				
$C^{12}H_2DGe^{74}H_3$	C_s	306		8 082.68 M	7 961.06 M				
$C^{12}H_3Ge^{76}D_3$	C_{3v}	307		7 930.11 M	7 930.11 M				
$C^{12}D_3Ge^{76}H_3$	C_{3v}	308		7 011.67 M	7 011.67 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
281	0.635 M	0. X	0. X		1239	25					
283				3							
284	0.651 M	0. X	0. X								

References:

ABC: 206, 248 D_J: D_{JK}: 248 κ: Δ:

μ: 248, 377 eQq: 248 V: 248 I: ω:

Add. Ref.: 205

The coupling parameter for species 299 and 303 is: $I_\alpha = 3.125$ amu Å^2. The coupling parameter for species 306 is: $I_\alpha = 6.251$ amu Å^2. Ref: 248.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Ge^{70}H_3$	281	1, 0← 0, 0	Ground							17 421.36	.10	248
		2, 0← 1, 0	Ground							34 842.46	.10	248
$C^{12}H_3Ge^{72}H_3$	282	1, 0← 0, 0	Ground							17 358.78	.10	248
		2, 0← 1, 0	Ground							34 717.54	.10	248
$C^{12}H_3Ge^{73}H_3$	283	1, 0← 0, 0	Ground				11/2		9/2	17 328.4	.10	248
		1, 0← 0, 0	Ground				7/2		9/2	17 328.4	.10	248
		1, 0← 0, 0	Ground				9/2		9/2	17 328.9	.10	248
		2, 1← 1, 1	Ground				13/2		11/2	34 656.75	.10	248
		2, 1← 1, 1	Ground				9/2		9/2	34 657.23	.10	248
		2, 1← 1, 1	Ground				11/2		9/2	34 657.23	.10	248
$C^{12}H_3Ge^{74}H_3$	284	1, 0← 0, 0	Ground	E	1					17 257.3	.10	248
		1, 0← 0, 0	Ground	A	1					17 258.8	.10	248
		1, 0← 0, 0	Ground							17 299.43	.10	248
		2, 0← 1, 0	Ground	E	1					34 514.5	.10	248
		2, 0← 1, 0	Ground	A	1					34 517.6	.10	248
		2, 0← 1, 0	Ground							34 598.62	.10	248
$C^{12}H_3Ge^{76}H_3$	285	1, 0← 0, 0	Ground							17 242.86	.10	248
		2, 0← 1, 0	Ground							34 485.90	.10	248
$C^{13}H_3Ge^{70}H_3$	286	1, 0← 0, 0	Ground							16 674.75	.10	248
		2, 0← 1, 0	Ground							33 349.30	.10	248
$C^{13}H_3Ge^{72}H_3$	287	1, 0← 0, 0	Ground							16 610.80	.10	248
		2, 0← 1, 0	Ground							33 221.62	.10	248
$C^{13}H_3Ge^{74}H_3$	288	1, 0← 0, 0	Ground	E	1					16 510.1	.10	248
		1, 0← 0, 0	Ground	A	1					16 511.5	.10	248
		1, 0← 0, 0	Ground							16 550.20	.10	248
		2, 0← 1, 0	Ground	E	1					33 020.2	.10	248
		2, 0← 1, 0	Ground	A	1					33 023.0	.10	248
		2, 0← 1, 0	Ground							33 100.38	.10	248
$C^{13}H_3Ge^{76}H_3$	289	1, 0← 0, 0	Ground							16 492.60	.10	248
		2, 0← 1, 0	Ground							32 984.82	.10	248
$C^{12}H_3Ge^{70}D_3$	291	1, 0← 0, 0	Ground							15 985.97	.10	248
		2, 0← 1, 0	Ground							31 972.02	.10	248
$C^{12}H_3Ge^{72}D_3$	292	1, 0← 0, 0	Ground							15 942.15	.10	248
		2, 0← 1, 0	Ground							31 884.25	.10	248
$C^{12}H_3Ge^{74}D_3$	293	1, 0← 0, 0	Ground							15 900.15	.10	248
		2, 0← 1, 0	Ground	E	1					31 729.5	.10	248
		2, 0← 1, 0	Ground	A	1					31 730.7	.10	248
		2, 0← 1, 0	Ground							31 800.35	.10	248
$C^{12}D_3Ge^{70}H_3$	294	1, 0← 0, 0	Ground							14 194.60	.10	248
		2, 0← 1, 0	Ground							28 389.10	.10	248
$C^{12}D_3Ge^{72}H_3$	295	1, 0← 0, 0	Ground							14 134.73	.10	248
		2, 0← 1, 0	Ground							28 269.15	.10	248

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3Ge^{74}H_3$	296	1, 0← 0, 0	Ground							14 077.80	.10	248
		1, 0← 0, 0	Ground							14 105.9	.10	248
		2, 0← 1, 0	Ground							28 155.20	.10	248
		2, 0← 1, 0	Ground							28 211.9	.10	248
$C^{12}H_3Ge^{70}H_2D$	297	2, 0, 2← 1, 0, 1	Ground	AE	0					33 827.32	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					33 987.35	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					34 115.77	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					33 541.74	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					33 670.44	.10	248
$C^{12}H_3Ge^{72}H_2D$	298	2, 0, 2← 1, 0, 1	Ground	AE	0					33 716.38	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					33 874.76	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					34 003.14	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					33 432.60	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					33 560.98	.10	248
$C^{12}H_3Ge^{74}H_2D$	299	2, 0, 2← 1, 0, 1	Ground	AE	0					33 610.80	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					33 767.66	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					33 895.92	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					33 328.63	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					33 767.80	.10	248
$C^{12}H_3Ge^{70}HD_2$	301	1, 0, 1← 0, 0, 0	Ground	AE	0					16 437.5	.10	248 [1]
		2, 0, 2← 1, 0, 1	Ground	AE	0					32 873.10	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					33 075.77	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					33 159.90	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					32 589.79	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					32 674.06	.10	248
$C^{12}H_3Ge^{72}HD_2$	302	1, 0, 1← 0, 0, 0	Ground	AE	0					16 388.2	.10	248 [1]
		2, 0, 2← 1, 0, 1	Ground	AE	0					32 774.60	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					32 975.24	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					33 059.35	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					32 492.95	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					32 577.29	.10	248
$C^{12}H_3Ge^{74}HD_2$	303	1, 0, 1← 0, 0, 0	Ground	AE	0					16 341.2	.10	248 [1]
		2, 0, 2← 1, 0, 1	Ground	AE	0					32 680.50	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					32 879.44	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					32 963.60	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					32 400.66	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					32 485.06	.10	248
$C^{12}H_2DGe^{70}H_3$	304	1, 0, 1← 0, 0, 0	Ground	AE	0					16 163.70	.10	248 [1]
		2, 0, 2← 1, 0, 1	Ground	AE	0					32 327.55	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					32 359.02	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					32 451.02	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					32 203.98	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					32 295.85	.10	248
$C^{12}H_2DGe^{72}H_3$	305	1, 0, 1← 0, 0, 0	Ground	AE	0					16 102.40	.10	248 [1]
		2, 0, 2← 1, 0, 1	Ground	AE	0					32 204.25	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					32 235.50	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					32 326.96	.10	248

1. For the ground torsional level, the $1_{01}\leftarrow 0_{00}$ and $2_{02}\leftarrow 1_{01}$ lines did not show significant A–E splitting.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2DGe^{72}H_3$	305	2, 1, 2← 1, 1, 1	Ground	A	0					32 081.95	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					32 173.40	.10	248
$C^{12}H_2DGe^{74}H_3$	306	1, 0, 1← 0, 0, 0	Ground	AE	0					16 043.80	.10	248 [1]
		2, 0, 2← 1, 0, 1	Ground	AE	0					32 087.40	.10	248 [1]
		2, 1, 1← 1, 1, 0	Ground	E	0					32 118.06	.10	248
		2, 1, 1← 1, 1, 0	Ground	A	0					32 209.10	.10	248
		2, 1, 2← 1, 1, 1	Ground	A	0					31 965.84	.10	248
		2, 1, 2← 1, 1, 1	Ground	AE	0					32 056.74	.10	248
$C^{12}H_3Ge^{76}D_3$	307	2, 0← 1, 0	Ground							31 720.45	.10	248
$C^{12}D_3Ge^{76}H_3$	308	2, 0← 1, 0	Ground							28 046.70	.10	248

1. For the ground torsional level, the $1_{01}\leftarrow 0_{00}$ and $2_{02}\leftarrow 1_{01}$ lines did not show significant A–E splitting.

CH_6Si $C_{3v}(C_{3v},C_{3v})$ ClH_3SiH_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Si^{28}H_3$	C_{3v}	311		10 968.96 M	10 968.96 M	−.001			
$C^{13}H_3Si^{28}H_3$	C_{3v}	312		10 606.52 M	10 606.52 M				
$C^{12}H_3Si^{29}H_3$	C_{3v}	313		10 885.54 M	10 885.54 M				
$C^{12}H_3Si^{30}H_3$	C_{3v}	314		10 806.53 M	10 806.53 M				
$C^{12}H_3Si^{28}D_3$	C_{3v}	315		9 622.78 M	9 622.78 M				
$C^{12}H_3Si^{29}D_3$	C_{3v}	316		9 572. M	9 572. M				
$C^{12}H_3Si^{30}D_3$	C_{3v}	317		9 525. M	9 525. M				
$C^{12}D_3Si^{28}D_3$	C_{3v}	318		8 079.03 M	8 079.03 M				
$C^{12}D_3Si^{29}D_3$	C_{3v}	319		8 028.81 M	8 028.81 M				
$C^{12}D_3Si^{30}D_3$	C_{3v}	321		7 981.12 M	7 981.12 M				
$C^{13}D_3Si^{28}D_3$	C_{3v}	322		7 889.68 M	7 889.68 M				
$C^{12}D_3Si^{28}H_3$	C_{3v}	323		9 119.98 M	9 119.98 M				
$C^{12}D_3Si^{29}H_3$	C_{3v}	324		9 040.82 M	9 040.82 M				
$C^{12}H_3Si^bH_2D$	C_s	325	46 750. M	10 671.21 M	10 270.68 M				
$C^{12}H_3Si^bHD_2$	C_s	326	39 717. M	10 229.72 M	9 822.25 M				
$C^{12}H_2DSi^bH_3$	C_s	327		10 346.48 M	10 148.29 M				
$C^{12}H_2DSi^bD_3$	C_s	328		9 100.18 M	8 948.85 M				
$C^{12}D_3Si^bH_2D$	C_s	329		8 874.74 M	8 597.77 M				
$C^{12}D_3Si^bHD_2$	C_s	331	31 300. M	8 533.77 M	8 250.06 M				
s-$C^{12}H_2DSi^bH_2D$	C_s	332		10 035.66 M	9 523.42 M				
a-$C^{12}H_2DSi^bH_2D$	C_1	333		9 962.01 M	9 645.77 M				
s-$C^{12}H_2DSi^bHD_2$	C_s	334		9 494.63 M	9 315.03 M				
a-$C^{12}H_2DSi^bHD_2$	C_1	335		9 615.96 M	9 153.46 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
311	0.73 M	0. X	0. X		1660						

References:

ABC: 28, 172 D_J: 172 D_{JK}: κ: Δ:

μ: 28, 172 eQq: V: 344 I: ω:

Add. Refs.: 90, 130, 141, 170, 287

$V_6 < 150$ cal/mol. Ref: 258.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_3Si^{28}H_3$	312	1, ← 0,								21 150.7		172
		1, ← 0,								21 213.04		172
$C^{12}D_3Si^{28}D_3$	318	1, ← 0,								16 085.3	.4	172
		1, ← 0,								16 125.04	.3	172
		1, ← 0,								16 158.06	.2	172
		2, ← 1,								32 170.41	.15	172
		2, ← 1,								32 239.63	.15	172
		2, ← 1,								32 316.07	.15	172
$C^{12}D_3Si^{29}D_3$	319	2, ← 1,								32 115.25	.15	172
$C^{12}D_3Si^{30}D_3$	321	2, ← 1,								31 924.49	.15	172
$C^{13}D_3Si^{28}D_3$	322	2, ← 1,								31 558.70	.3	172
$C^{12}D_3Si^{28}H_3$	323	1, ← 0,								18 150.0	.3	172
		1, ← 0,								18 192.81	.2	172
		1, ← 0,								18 239.95	.15	172
$C^{12}D_3Si^{29}H_3$	324	1, ← 0,								18 081.65	.3	172
$C^{12}H_3Si^{b}H_2D$	325	1, 0, 1← 0, 0, 0								20 801.74		172
		1, 0, 1← 0, 0, 0								20 906.36	.1	172
		1, 0, 1← 0, 0, 0								20 941.87	.1	172
		2, 0, 2← 1, 0, 1								41 758.92		172
		2, 0, 2← 1, 0, 1								41 880.10	.4	172
		2, 1, 1← 1, 1, 0		E	0					42 264.12	.4	172
		2, 1, 1← 1, 1, 0		A	0					42 283.52	.2	172
		2, 1, 2← 1, 1, 1		A	0					41 482.84	.2	172
		2, 1, 2← 1, 1, 1		E	0					41 502.14	.4	172
		8, 1, 7← 8, 1, 8								14 405.90	.1	172
		9, 1, 8← 9, 1, 9								17 998.95	.2	172
		10, 1, 9←10, 1,10								21 986.66		172
		11, 1,10←11, 1,11								26 365.07		172
		12, 1,11←12, 1,12								31 130.43		172
		Not Reported								14 404.95		172
$C^{12}H_3Si^{b}HD_2$	326	1, 0, 1← 0, 0, 0								19 995.56	.1	172
		1, 0, 1← 0, 0, 0								20 052.10	.1	172
		2, 0, 2← 1, 0, 1								40 100.00	.4	172
		2, 1, 1← 1, 1, 0		E	0					40 503.64	.4	172
		2, 1, 1← 1, 1, 0		A	0					40 510.98	.4	172
		2, 1, 2← 1, 1, 1		A	0					39 696.34	.2	172
		2, 1, 2← 1, 1, 1		E	0					39 703.74	.2	172
		8, 1, 7← 8, 1, 8								14 651.55	.1	172
		9, 1, 8← 9, 1, 9								18 303.84	.1	172
		10, 1, 9←10, 1,10								22 353.73	.2	172
		11, 1,10←11, 1,11								26 797.15	.2	172
		12, 1,11←12, 1,12								31 627.61	.2	172
		Not Reported								14 649.60	.2	172
		Not Reported								14 663.02		172

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2DSi^bH_3$	327	1, 0, 1← 0, 0, 0								20 437.6		172
		1, 0, 1← 0, 0, 0								20 494.80		172
		2, 0, 2← 1, 0, 1								40 988.76	.4	172
		2, 1, 1← 1, 1, 0		E	0					41 155.38	.2	172
		2, 1, 1← 1, 1, 0		A	0					41 187.62	.2	172
		2, 1, 2← 1, 1, 1		A	0					40 791.24	.2	172
		2, 1, 2← 1, 1, 1		E	0					40 823.44	.2	172
$C^{12}H_2DSi^bD_3$	328	1, 0, 1← 1, 0, 0								18 002.90	.2	172
		1, 0, 1← 1, 0, 0								18 049.08	.1	172
		2, 0, 2← 1, 0, 1								36 097.35	.2	172
		2, 1, 1← 1, 1, 0		E	0					36 246.17	.3	172
		2, 1, 1← 1, 1, 0		A	0					36 249.26	.3	172
		2, 1, 2← 1, 1, 1		A	0					35 873.39	.3	172
		2, 1, 2← 1, 1, 1		E	0					35 946.59	.2	172
		2, 1, 2← 1, 1, 1								35 950.03	.2	172
$C^{12}D_3Si^bH_2D$	329	1, 0, 1← 0, 0, 0								17 428.89	.3	172
		1, 0, 1← 0, 0, 0								17 472.57	.1	172
		2, 0, 2← 1, 0, 1								34 942.63	.2	172
		2, 1, 1← 1, 1, 0		A	0					35 221.73	.2	172
		2, 1, 2← 1, 1, 1		A	0					34 667.79	.2	172
$C^{12}D_3Si^bHD_2$	331	1, 0, 1← 0, 0, 0								16 743.20		172
		1, 0, 1← 0, 0, 0								16 783.88	.2	172
		2, 0, 2← 1, 0, 1								33 323.		172
		2, 0, 2← 1, 0, 1								33 409.81	.2	172
		2, 0, 2← 1, 0, 1								33 483.80	.2	172
		2, 0, 2← 1, 0, 1								33 565.07	.2	172
		2, 1, 1← 1, 1, 0		A	0					33 851.17	.2	172
		2, 1, 2← 1, 1, 1								33 213.00	.2	172
		2, 1, 2← 1, 1, 1		A	0					33 283.75	.2	172
		8, 1, 7← 8, 1, 8								10 208.20	.2	172
		9, 1, 8← 9, 1, 9								12 754.31	.2	172
		10, 1, 9←10, 1,10								15 579.07	.2	172
		11, 1,10←11, 1,11								18 679.69	.3	172
		12, 1,11←12, 1,12								22 053.50	.3	172
		14, 1,13←14, 1,14								29 600.50	1.	172
		15, 1,14←15, 1,15								33 759.17	.4	172
		Not Reported								33 839.0	.4	172
s-$C^{12}H_2DSi^bH_2D$	332	1, , ← 0, ,								19 559.2		172
		2, 0, 2← 1, 0, 1								39 111.84		172
		2, 1, 1← 1, 1, 0								39 629.92		172
		2, 1, 2← 1, 1, 1								38 605.44		172
a-$C^{12}H_2DSi^bH_2D$	333	1, , ← 0, ,								19 607.85		172
		2, 0, 2← 1, 0, 1								39 213.18		172
		2, 1, 1← 1, 1, 0								39 531.54		172
		2, 1, 2← 1, 1, 1								38 899.06		172
s-$C^{12}H_2DSi^bHD_2$	334	1, , ← 0, ,								18 809.74	.1	172
		2, 0, 2← 1, 0, 1								37 618.28		172
		2, 1, 1← 1, 1, 0								37 798.60		172
		2, 1, 2← 1, 1, 1								37 439.40		172
a-$C^{12}H_2DSi^bHD_2$	335	1, , ← 0, ,								18 720.19	.1	172
		1, , ← 0, ,								18 769.49	.1	172
		2, 0, 2← 1, 0, 1								37 533.0		172
		2, 1, 1← 1, 1, 0								38 001.08		172
		2, 1, 2← 1, 1, 1								37 076.08		172

CH_6Sn $C_{3v}(C_{3v},C_{3v})$ CH_3SnH_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3Sn^{118}H_3$	C_{3v}	341		6906.35[1] M					

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
341	0.68 M	0. X	0. X		650	30					

1. Cahill and Butcher call this rotational constant B_v, although they do not indicate that any non-torsional mode was excited.

References:

ABC: 314 D_J: D_{JK}: κ: Δ:

μ: 40 eQq: V: 314 I: ω:

Methyltin

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3Sn^{118}H_3$	341	1, ← 0,	Ground	A	3					13 749.70		314
		1, ← 0,	Ground	E	3					13 755.22		314
		1, ← 0,	Ground	A	2					13 757.87		314
		1, ← 0,	Ground	E	2					13 759.66		314
		1, ← 0,	Ground	E	1					13 775.97		314
		1, ← 0,	Ground	A	1					13 778.92		314
		1, ← 0,	Ground		0					13 800.31		314
		2, ← 1,	Ground							27 558.79	.10	40
		2, ← 1,	Ground							27 600.80	.10	40
$C^{12}H_3Sn^{116}H_3$	342	1, ← 0,	Ground	A	3					13 769.94		314
		1, ← 0,	Ground	A	2					13 778.22		314
		1, ← 0,	Ground	E	1					13 796.43		314
		1, ← 0,	Ground	A	1					13 799.38		314
		1, ← 0,	Ground		0					13 820.87		314
		2, ← 1,	Ground							27 641.99	.10	40
$C^{12}H_3Sn^{117}H_3$	343	1, ← 0,	Ground	A	2					13 767.81		314
		1, ← 0,	Ground	E	1					13 786.22		314
		1, ← 0,	Ground	A	1					13 789.11		314
		1, ← 0,	Ground		0					13 810.73		314
		2, ← 1,	Ground							27 621.20	.10	40
$C^{12}H_3Sn^{119}H_3$	344	1, ← 0,	Ground	A	2					13 747.81		314
		1, ← 0,	Ground	E	1					13 765.89		314
		1, ← 0,	Ground	A	1					13 768.87		314
		1, ← 0,	Ground		0					13 790.49		314
		2, ← 1,	Ground							27 580.52	.10	40
$C^{12}H_3Sn^{120}H_3$	345	1, ← 0,	Ground	A	3					13 729.81		314
		1, ← 0,	Ground	E	3					13 735.34		314
		1, ← 0,	Ground	A	2					13 737.98		314
		1, ← 0,	Ground	E	1					13 756.27		314
		1, ← 0,	Ground	A	1					13 759.20		314
		1, ← 0,	Ground		0					13 780.72		314
		2, ← 1,	Ground							27 517.58	.10	40
		2, ← 1,	Ground							27 560.69	.10	40
$C^{12}H_3Sn^{122}H_3$	346	1, ← 0,	Ground	E	1					13 736.90		314
		1, ← 0,	Ground	A	1					13 740.01		314
		1, ← 0,	Ground		0					13 761.24		314
$C^{12}H_3Sn^{124}H_3$	347	1, ← 0,	Ground	A	1					13 721.1		314
		1, ← 0,	Ground		0					13 742.56		314

C_2H_3BrO $C_s(C_{3v},C_s)$ CH_3COBr

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}O^{16}Br^{79}$	C_s	351	10 126.35 M	3 027.02 M	2 362.52 M				
$C^{12}H_3C^{12}O^{16}Br^{81}$	C_s	352	10 126.11 M	3 001.64 M	2 347.12 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
351	2.43 T		0. X	−770	1306						
352					1304						

References:

ABC: 289 D_J: D_{JK}: κ: Δ:

μ: 395 eQq: 289 V: 289 I: ω:

For species 351, the quadrupole coupling constants are $\chi_{aa}=460\pm3$ MHz, $\chi_{bb}=-277\pm1$ MHz, $\chi_{cc}=-183\pm3$ MHz, eQq = −770 MHz, and the coupling parameter is $I_\alpha=3.14$ amu Å². For species 352, the quadrupole coupling constants are $\chi_{aa}=385\pm3$ MHz, $\chi_{bb}=-232\pm1$ MHz, $\chi_{cc}=-153\pm3$ MHz, and the coupling parameter is $I_\alpha=3.14$ amu Å². Ref: 289.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Br^{79}$	351	1, 1, 1← 0, 0, 0	Ground				3/2		3/2	12 433.58	.15	289
		1, 1, 1← 0, 0, 0	Ground				5/2		3/2	12 502.61	.15	289
		1, 1, 1← 0, 0, 0	Ground				1/2		3/2	12 558.12	.15	289
		2, 1, 2← 1, 0, 1	Ground				5/2		3/2	17 154.98	.15	289
		2, 1, 2← 1, 0, 1	Ground				7/2		5/2	17 223.65	.15	289
		3, 1, 3← 2, 0, 2	Ground				7/2		5/2	21 592.05	.15	289
		3, 1, 3← 2, 0, 2	Ground				9/2		7/2	21 631.72	.15	289
		3, 1, 3← 2, 0, 2	Ground				5/2		3/2	21 638.05	.15	289
		3, 1, 3← 2, 0, 2	Ground				3/2		1/2	21 677.89	.15	289
		4, 1, 4← 3, 0, 3	Ground				9/2		7/2	25 756.54	.15	289
		4, 1, 4← 3, 0, 3	Ground				7/2		5/2	25 778.50	.15	289
		4, 1, 4← 3, 0, 3	Ground				11/2		9/2	25 783.12	.15	289
		4, 1, 4← 3, 0, 3	Ground				5/2		3/2	25 805.56	.15	289
		4, 1, 3← 3, 1, 2	Ground	E	0		11/2		9/2	22 786.79	.15	289
		4, 1, 3← 3, 1, 2	Ground	A	0		11/2		9/2	22 787.47	.15	289
		4, 1, 3← 3, 1, 2	Ground				5/2		3/2	22 794.65		289
		4, 1, 3← 3, 1, 2	Ground	E	0		9/2		7/2	22 797.44	.15	289
		4, 1, 3← 3, 1, 2	Ground	A	0		9/2		7/2	22 797.96	.15	289
		4, 1, 3← 3, 1, 2	Ground	E	0		7/2		5/2	22 803.90	.15	289
		4, 1, 3← 3, 1, 2	Ground	A	0		7/2		5/2	22 805.15	.15	289
		4, 1, 4← 3, 1, 3	Ground				11/2		9/2	20 139.43	.15	289
		4, 1, 4← 3, 1, 3	Ground				5/2		3/2	20 143.77	.15	289
		4, 1, 4← 3, 1, 3	Ground				9/2		7/2	20 150.49	.15	289
		4, 1, 4← 3, 1, 3	Ground				7/2		5/2	20 154.92	.15	289
		5, 0, 5← 4, 0, 4	Ground				11/2		9/2	26 108.30	.15	289
		5, 0, 5← 4, 0, 4	Ground				13/2		11/2	26 111.40	.15	289
		5, 0, 5← 4, 0, 4	Ground				9/2		7/2	26 116.67	.15	289
		5, 0, 5← 4, 0, 4	Ground				7/2		5/2	26 119.37	.15	289
		5, 0, 5← 4, 1, 4	Ground				13/2		11/2	21 450.87	.15	289
		5, 0, 5← 4, 1, 4	Ground				7/2		5/2	21 450.87	.15	289
		5, 0, 5← 4, 1, 4	Ground				11/2		9/2	21 471.39	.15	289
		5, 0, 5← 4, 1, 4	Ground				9/2		7/2	21 471.39	.15	289
		5, 1, 5← 4, 1, 4	Ground				13/2		11/2	25 106.53	.15	289
		5, 1, 5← 4, 1, 4	Ground				7/2		5/2	25 110.84	.15	289
		5, 1, 5← 4, 1, 4	Ground				11/2		9/2	25 111.43	.15	289
		5, 1, 5← 4, 1, 4	Ground				9/2		7/2	25 115.74	.15	289
		7, 1, 6← 7, 0, 7	Ground	E	0		11/2		11/2	20 171.49	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		11/2		11/2	20 174.67	.15	289
		7, 1, 6← 7, 0, 7	Ground	E	0		17/2		17/2	20 174.67	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		17/2		17/2	20 177.63	.15	289
		7, 1, 6← 7, 0, 7	Ground	E	0		13/2		13/2	20 186.19	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		13/2		13/2	20 189.13	.15	289
		7, 1, 6← 7, 0, 7	Ground	E	0		15/2		15/2	20 189.13	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		15/2		15/2	20 192.05	.15	289
		8, 1, 7← 8, 0, 8	Ground	E	0		13/2		13/2	24 442.49	.15	289
		8, 1, 7← 8, 0, 8	Ground	A	0		13/2		13/2	24 445.67		289
		8, 1, 7← 8, 0, 8	Ground	E	0		19/2		19/2	24 445.67		289
		8, 1, 7← 8, 0, 8	Ground	A	0		19/2		19/2	24 449.17	.15	289
		8, 1, 7← 8, 0, 8	Ground	E	0		15/2		15/2	24 458.58	.15	289
		8, 1, 7← 8, 0, 8	Ground	E	0		17/2		17/2	24 461.41	.15	289

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Br^{79}$	351	8, 1, 7← 8, 0, 8	Ground	A	0		15/2		15/2	24 462.07	.15	289
		8, 1, 7← 8, 0, 8	Ground	A	0		17/2		17/2	24 464.90	.15	289
		8, 3, 5← 8, 2, 6	Ground				17/2		17/2	32 602.01	.15	289
		8, 3, 5← 8, 2, 6	Ground				15/2		15/2	32 607.52	.15	289
		8, 3, 5← 8, 2, 6	Ground				19/2		19/2	32 633.34	.15	289
		8, 3, 5← 8, 2, 6	Ground				13/2		13/2	32 638.93	.15	289
		9, 2, 7← 9, 1, 8	Ground	E	0					20 621.91		289
		9, 2, 7← 9, 1, 8	Ground	A	0					20 623.67		289
		9, 3, 6← 9, 2, 7	Ground				19/2		19/2	31 115.92	.15	289
		9, 3, 6← 9, 2, 7	Ground				17/2		17/2	31 119.74	.15	289
		9, 3, 6← 9, 2, 7	Ground				21/2		21/2	31 141.07	.15	289
		9, 3, 6← 9, 2, 7	Ground				15/2		15/2	31 145.05	.15	289
		10, 2, 8←10, 1, 9	Ground	E	0		17/2		17/2	22 722.86	.15	289
		10, 2, 8←10, 1, 9	Ground	E	0		23/2		23/2	22 723.66	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		17/2		17/2	22 725.54	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		23/2		23/2	22 726.34	.15	289
		10, 2, 8←10, 1, 9	Ground	E	0		19/2		19/2	22 727.32	.15	289
		10, 2, 8←10, 1, 9	Ground	E	0		21/2		21/2	22 727.85	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		19/2		19/2	22 729.99	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		21/2		21/2	22 730.54	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		19/2		19/2	25 637.62	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		25/2		25/2	25 638.65	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		19/2		19/2	25 641.10	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		25/2		25/2	25 642.22	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		21/2		21/2	25 645.62	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		23/2		23/2	25 646.50	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		21/2		21/2	25 649.20	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		23/2		23/2	25 650.34	.15	289
		11, 3, 8←11, 2, 9	Ground				23/2		23/2	28 710.85	.15	289
		11, 3, 8←11, 2, 9	Ground				21/2		21/2	28 712.58	.15	289
		11, 3, 8←11, 2, 9	Ground				25/2		25/2	28 725.02	.15	289
		11, 3, 8←11, 2, 9	Ground				19/2		19/2	28 726.92	.15	289
		12, 3, 9←12, 2,10	Ground				25/2		25/2	28 198.0		289
		12, 3, 9←12, 2,10	Ground				23/2		23/2	28 198.0		289
		12, 3, 9←12, 2,10	Ground				27/2		27/2	28 208.0		289
		12, 3, 9←12, 2,10	Ground				21/2		21/2	28 208.0		289
$C^{12}H_3C^{12}O^{16}Br^{81}$	352	1, 1, 1← 0, 0, 0	Ground				3/2		3/2	12 426.91	.15	289
		1, 1, 1← 0, 0, 0	Ground				5/2		3/2	12 484.78	.15	289
		1, 1, 1← 0, 0, 0	Ground				1/2		3/2	12 531.19	.15	289
		2, 1, 2← 1, 0, 1	Ground				3/2		3/2	17 090.78	.15	289
		2, 1, 2← 1, 0, 1	Ground				5/2		3/2	17 117.81	.3	289
		2, 1, 2← 1, 0, 1	Ground				7/2		5/2	17 175.72	.15	289
		3, 1, 3← 2, 0, 2	Ground				7/2		5/2	21 524.02	.15	289
		3, 1, 3← 2, 0, 2	Ground				9/2		7/2	21 557.11	.15	289
		3, 1, 3← 2, 0, 2	Ground				5/2		3/2	21 562.60	.15	289
		3, 1, 3← 2, 0, 2	Ground				3/2		1/2	21 595.04	.15	289
		4, 0, 4← 3, 0, 3	Ground				9/2		7/2	20 971.00	.15	289
		4, 0, 4← 3, 0, 3	Ground				11/2		9/2	20 973.66	.15	289
		4, 0, 4← 3, 0, 3	Ground				7/2		5/2	20 982.43	.15	289

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Br^{81}$	352	4, 0, 4← 3, 0, 3	Ground				5/2		3/2	20 984.47	.15	289
		4, 1, 4← 3, 0, 3	Ground				9/2		7/2	25 662.47	.15	289
		4, 1, 4← 3, 0, 3	Ground				7/2		5/2	25 680.83	.15	289
		4, 1, 4← 3, 0, 3	Ground				11/2		9/2	25 684.46	.15	289
		4, 1, 4← 3, 0, 3	Ground				5/2		3/2	25 703.40	.15	289
		4, 1, 3← 3, 1, 2	Ground	A	0		11/2		9/2	22 606.54	.15	289
		4, 1, 3← 3, 1, 2	Ground				5/2		3/2	22 614.59	.15	289
		4, 1, 3← 3, 1, 2	Ground	A	0		9/2		7/2	22 616.98	.15	289
		4, 1, 3← 3, 1, 2	Ground	A	0		7/2		5/2	22 623.21	.15	289
		4, 1, 4← 3, 1, 3	Ground				11/2		9/2	19 999.26	.15	289
		4, 1, 4← 3, 1, 3	Ground				5/2		3/2	20 003.13	.15	289
		4, 1, 4← 3, 1, 3	Ground				9/2		7/2	20 007.96	.15	289
		4, 1, 4← 3, 1, 3	Ground				7/2		5/2	20 012.11	.15	289
		5, 0, 5← 4, 0, 4	Ground				11/2		9/2	25 930.24	.15	289
		5, 0, 5← 4, 0, 4	Ground				13/2		11/2	25 932.46	.15	289
		5, 0, 5← 4, 0, 4	Ground				9/2		7/2	25 936.96	.15	289
		5, 0, 5← 4, 0, 4	Ground				7/2		5/2	25 938.87	.15	289
		5, 0, 5← 4, 1, 4	Ground				13/2		11/2	21 220.85	.15	289
		5, 0, 5← 4, 1, 4	Ground				7/2		5/2	21 220.85	.15	289
		5, 0, 5← 4, 1, 4	Ground				11/2		9/2	21 238.52	.15	289
		5, 0, 5← 4, 1, 4	Ground				9/2		7/2	21 238.52	.15	289
		5, 1, 5← 4, 0, 4	Ground				11/2		9/2	29 628.40	.15	289
		5, 1, 5← 4, 0, 4	Ground				9/2		7/2	29 638.95	.15	289
		5, 1, 5← 4, 0, 4	Ground				13/2		11/2	29 644.39	.15	289
		5, 1, 5← 4, 0, 4	Ground				7/2		5/2	29 655.20	.15	289
		5, 1, 5← 4, 1, 4	Ground				13/2		11/2	24 932.92	.15	289
		5, 1, 5← 4, 1, 4	Ground				7/2		5/2	24 936.55	.15	289
		5, 1, 5← 4, 1, 4	Ground				11/2		9/2	24 937.28	.15	289
		5, 1, 5← 4, 1, 4	Ground				9/2		7/2	24 940.70	.15	289
		6, 0, 6← 5, 1, 5	Ground				15/2		13/2	27 041.92		289
		6, 0, 6← 5, 1, 5	Ground				9/2		7/2	27 041.92		289
		6, 0, 6← 5, 1, 5	Ground				13/2		11/2	27 053.88		289
		6, 0, 6← 5, 1, 5	Ground				11/2		9/2	27 053.88		289
		7, 1, 6← 7, 0, 7	Ground	E	0		11/2		11/2	19 966.22	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		11/2		11/2	19 969.09	.15	289
		7, 1, 6← 7, 0, 7	Ground	E	0		17/2		17/2	19 969.09	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		17/2		17/2	19 971.96	.15	289
		7, 1, 6← 7, 0, 7	Ground	E	0		13/2		13/2	19 978.80	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		13/2		13/2	19 981.44	.15	289
		7, 1, 6← 7, 0, 7	Ground	E	0		15/2		15/2	19 981.44	.15	289
		7, 1, 6← 7, 0, 7	Ground	A	0		15/2		15/2	19 984.18	.15	289
		8, 1, 7← 8, 0, 8	Ground	E	0		13/2		13/2	24 170.70	.15	289
		8, 1, 7← 8, 0, 8	Ground	E	0		19/2		19/2	24 173.27	.15	289
		8, 1, 7← 8, 0, 8	Ground	A	0		13/2		13/2	24 174.40	.15	289
		8, 1, 7← 8, 0, 8	Ground	A	0		19/2		19/2	24 176.97	.15	289
		8, 1, 7← 8, 0, 8	Ground	E	0		15/2		15/2	24 184.13	.15	289
		8, 1, 7← 8, 0, 8	Ground	E	0		17/2		17/2	24 186.53	.15	289
		8, 1, 7← 8, 0, 8	Ground	A	0		15/2		15/2	24 187.65	.15	289
		8, 1, 7← 8, 0, 8	Ground	A	0		17/2		17/2	24 190.15	.15	289
		8, 3, 5← 8, 2, 6	Ground				17/2		17/2	32 804.90	.15	289

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Br^{81}$	352	8, 3, 5← 8, 2, 6	Ground				15/2		15/2	32 809.49	.15	289
		8, 3, 5← 8, 2, 6	Ground				19/2		19/2	32 830.87	.15	289
		8, 3, 5← 8, 2, 6	Ground				13/2		13/2	32 835.67	.15	289
		9, 2, 7← 9, 1, 8	Ground	E	0					20 541.46		289
		9, 2, 7← 9, 1, 8	Ground	A	0					20 543.00		289
		9, 3, 6← 9, 2, 7	Ground				19/2		19/2	31 326.92	.15	289
		9, 3, 6← 9, 2, 7	Ground				17/2		17/2	31 330.21	.15	289
		9, 3, 6← 9, 2, 7	Ground				21/2		21/2	31 348.15	.15	289
		9, 3, 6← 9, 2, 7	Ground				15/2		15/2	31 351.55	.15	289
		10, 2, 8←10, 1, 9	Ground	E	0		17/2		17/2	22 561.01	.15	289
		10, 2, 8←10, 1, 9	Ground	E	0		23/2		23/2	22 561.63	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		17/2		17/2	22 563.55	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		23/2		23/2	22 564.33		289
		10, 2, 8←10, 1, 9	Ground	E	0		19/2		19/2	22 564.33		289
		10, 2, 8←10, 1, 9	Ground	E	0		21/2		21/2	22 564.77	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		19/2		19/2	22 566.91	.15	289
		10, 2, 8←10, 1, 9	Ground	A	0		21/2		21/2	22 567.38	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		19/2		19/2	25 379.89	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		25/2		25/2	25 380.83	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		19/2		19/2	25 383.41	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		25/2		25/2	25 384.32	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		21/2		21/2	25 386.35	.15	289
		11, 2, 9←11, 1,10	Ground	E	0		23/2		23/2	25 387.14	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		21/2		21/2	25 389.77	.15	289
		11, 2, 9←11, 1,10	Ground	A	0		23/2		23/2	25 390.60	.15	289
		11, 3, 8←11, 2, 9	Ground				23/2		23/2	28 876.40	.4	289
		11, 3, 8←11, 2, 9	Ground				21/2		21/2	28 877.80	.4	289
		11, 3, 8←11, 2, 9	Ground				25/2		25/2	28 889.0	.4	289
		11, 3, 8←11, 2, 9	Ground				19/2		19/2	28 890.4	.4	289
		12, 3, 9←12, 2,10	Ground				25/2		25/2	28 305.51		289
		12, 3, 9←12, 2,10	Ground				23/2		23/2	28 305.51		289
		12, 3, 9←12, 2,10	Ground				21/2		21/2	28 313.04		289
		12, 3, 9←12, 2,10	Ground				27/2		27/2	28 313.04		289

C_2H_3ClO $C_s(C_{3v},C_s)$ CH_3COCl

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}O^{16}Cl^{35}$	C_s	361	10 162.39 M	4 946.66 M	3 393.07 M				
$C^{12}H_3C^{12}O^{16}Cl^{37}$	C_s	362	10 160.60 M	4 808.74 M	3 327.40 M				
$C^{12}D_3C^{12}O^{16}Cl^{35}$	C_s	363	8 758.77 M	4 532.73 M	3 098.77 M				
$C^{12}D_3C^{12}O^{16}Cl^{37}$	C_s	364	8 753.45 M	4 408.08 M	3 039.17 M				
s-$C^{12}H_2DC^{12}O^{16}Cl^{35}$	C_s	365	9 973.64 M	4 691.78 M	3 252.28 M				
a-$C^{12}H_2DC^{12}O^{16}Cl^{35}$	C_1	366	9 444.93 M	4 867.07 M	3 303.13 M				
$C^{13}H_3C^{12}O^{16}Cl^{35}$	C_s	367	9 894.47 M	4 868.35 M	3 326.21 M				
$C^{13}H_3C^{12}O^{16}Cl^{37}$	C_s	368	9 889.14 M	4 731.58 M	3 261.38 M				
$C^{12}H_3C^{13}O^{16}Cl^{35}$	C_s	369	10 159.49 M	4 932.06 M	3 385.97 M				
$C^{12}H_3C^{13}O^{16}Cl^{37}$	C_s	371							
$C^{12}H_3C^{12}O^{18}Cl^{35}$	C_s	372	9 623.48 M	4 841.02 M	3 282.56 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
361	2.72 T		0. X		1296	30					
362					1296	30					
367					1287						
368					1301						
369					1283						
371					1296						
372					1315						

References:

ABC: 337, 384 D_J: D_{JK}: κ: Δ:

μ: 393 eQq: V: 337 I: ω:

Add. Ref.: 153

Id. No.	Quadrupole Coupling Constants χ_{aa}(MHz)	χ_{bb}(MHz)	χ_{cc}(MHz)	Coupling Parameter I_α (amu Å^2).
361	−58.0	36.4	21.6	3.1158
362	−45.5	28.5	17.0	3.1158
363	−53.2	31.7	21.5	3.1158
364	−42.9	25.4	17.5	3.1158
367–372				3.1158

Ref: 337.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Cl^{35}$	361	2, 1, 2← 1, 0, 1	Ground	AE	0		3/2		1/2	20 327.30	.2	337
		2, 1, 2← 1, 0, 1	Ground	AE	0		1/2		1/2	20 332.60	.2	337
		2, 1, 2← 1, 0, 1	Ground	AE	0		5/2		5/2	20 334.80	.2	337
		2, 1, 2← 1, 0, 1	Ground	AE	0		7/2		5/2	20 340.25	.2	337
		2, 1, 2← 1, 0, 1	Ground	AE	0		5/2		3/2	20 349.25	.2	337
		2, 1, 2← 1, 0, 1	Ground	AE	0		3/2		3/2	20 353.25	.2	337
		2, 2, 1← 2, 1, 2	Ground							20 298.0	.2	384
		2, 2, 1← 2, 1, 2	Ground							20 305.0	.2	384
		3, 0, 3← 2, 1, 2	Ground	AE	0		7/2		5/2	19 926.80	.2	337
		3, 0, 3← 2, 1, 2	Ground	AE	0		5/2		3/2	19 928.25	.2	337
		3, 0, 3← 2, 1, 2	Ground	AE	0		5/2		5/2	19 932.10	.2	337
		3, 0, 3← 2, 1, 2	Ground	AE	0		9/2		7/2	19 934.00	.2	337
		3, 0, 3← 2, 1, 2	Ground	AE	0		3/2		1/2	19 936.00	.2	337
		3, 0, 3← 2, 1, 2	Ground	AE	0		3/2		3/2	19 941.80	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		7/2		7/2	26 467.75	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		3/2		1/2	26 471.05	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		5/2		3/2	26 476.55	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		9/2		7/2	26 476.55	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		7/2		5/2	26 481.53	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		5/2		5/2	26 485.20	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		3/2		3/2	26 485.20	.2	337
		3, 2, 2← 3, 1, 3	Ground							22 800.0	.2	384
		3, 2, 2← 3, 1, 3	Ground							22 804.3	.2	384
		4, 0, 4← 3, 1, 3	Ground	E	0		7/2		5/2	28 278.10	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		9/2		7/2	28 278.10	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		9/2		7/2	28 278.78	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		7/2		5/2	28 278.78	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		11/2		9/2	28 281.08	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		5/2		3/2	28 281.08	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		5/2		3/2	28 281.76	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		11/2		9/2	28 281.76	.2	337
		4, 1, 3← 4, 0, 4	Ground							16 743.0	.2	384
		4, 1, 3← 4, 0, 4	Ground							16 753.0	.2	384
		4, 1, 3← 4, 0, 4	Ground							16 755.0	.2	384
		4, 2, 2← 4, 1, 3	Ground							14 810.8	.2	384
		4, 2, 2← 4, 1, 3	Ground							14 814.2	.2	384
		4, 2, 2← 4, 1, 3	Ground							14 817.2	.2	384
		4, 2, 3← 4, 1, 4	Ground	E	0		5		5	26 181.00	.2	337
		4, 2, 3← 4, 1, 4	Ground	E	0		11		11	26 182.60	.2	337
		4, 2, 3← 4, 1, 4	Ground	A	0		5		5	26 182.60	.2	337
		4, 2, 3← 4, 1, 4	Ground	A	0		11		11	26 183.95	.2	337
		4, 2, 3← 4, 1, 4	Ground	E	0		7		7	26 185.50	.2	337
		4, 2, 3← 4, 1, 4	Ground	E	0		9		9	26 186.80	.2	337
		4, 2, 3← 4, 1, 4	Ground	A	0		7		7	26 186.80	.2	337
		4, 2, 3← 4, 1, 4	Ground	A	0		9		9	26 188.30	.2	337
		5, 1, 4← 5, 0, 5	Ground	E	0		9/2		9/2	23 090.50	.2	337
		5, 1, 4← 5, 0, 5	Ground	E	0		11/2		11/2	23 090.50	.2	337
		5, 1, 4← 5, 0, 5	Ground	E	0		13/2		13/2	23 092.30	.2	337
		5, 1, 4← 5, 0, 5	Ground	E	0		7/2		7/2	23 092.30	.2	337
		5, 1, 4← 5, 0, 5	Ground	A	0		9/2		9/2	23 095.25	.2	337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Cl^{35}$	361	5, 1, 4← 5, 0, 5	Ground	A	0		11/2		11/2	23 095.25	.2	337
		5, 1, 4← 5, 0, 5	Ground	A	0		7/2		7/2	23 097.14	.2	337
		5, 1, 4← 5, 0, 5	Ground	A	0		13/2		13/2	23 097.14	.2	337
		5, 2, 3← 5, 1, 4	Ground							16 083.2	.2	384
		5, 2, 3← 5, 1, 4	Ground							16 085.0	.2	384
		5, 2, 3← 5, 1, 4	Ground							16 086.8	.2	384
		5, 3, 2← 5, 2, 3	Ground	AE	0		7/2		7/2	25 150.65	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		13/2		13/2	25 153.00	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		9/2		9/2	25 159.20	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		11/2		11/2	25 161.60	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		15/2		15/2	19 125.31	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		9/2		9/2	19 125.31	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		13/2		13/2	19 125.31	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		11/2		11/2	19 125.31	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		15/2		15/2	19 128.55	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		13/2		13/2	19 128.55	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		11/2		11/2	19 128.55	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		9/2		9/2	19 128.55	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		9/2		9/2	23 260.30	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		15/2		15/2	23 261.50	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		11/2		11/2	23 265.75	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		13/2		13/2	23 267.00	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		15/2		15/2	24 086.30	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		13/2		13/2	24 086.30	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		11		11	24 087.55	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		17/2		17/2	24 087.55	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		15		15	24 091.40	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		13		13	24 091.40	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		11		11	24 092.65	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		17		17	24 092.65	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		11		11	22 344.40	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		17		17	22 345.20	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		11		11	22 345.20	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		17		17	22 346.02	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		13		13	22 347.65	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		15		15	22 348.40	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		13		13	22 348.40	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		15		15	22 349.23	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		13		13	23 073.27	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		19		19	23 073.27	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		15		15	23 074.50	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		17		17	23 074.50	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		13		13	23 075.56	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		19		19	23 075.56	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		15/2		15/2	23 076.80	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		17/2		17/2	23 076.80	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		19/2		19/2	25 860.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		17/2		17/2	25 860.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		21/2		21/2	25 860.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		15/2		15/2	25 860.85	.2	337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Cl^{35}$	361	9, 3, 6← 9, 2, 7	Ground	A	0		19/2		19/2	25 865.30	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		17/2		17/2	25 865.30	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		21/2		21/2	25 865.30	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		15/2		15/2	25 865.30	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		21/2		21/2	30 836.85	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		19/2		19/2	30 836.85	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		23/2		23/2	30 837.95	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		17/2		17/2	30 837.95	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		21/2		21/2	30 843.67	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		19/2		19/2	30 843.67	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		23/2		23/2	30 844.77	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		17/2		17/2	30 844.77	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		19/2		19/2	29 817.85	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		25/2		25/2	29 817.85	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		21/2		21/2	29 819.00	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		23/2		23/2	29 819.00	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		19/2		19/2	29 820.30	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		25/2		25/2	29 820.30	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		21/2		21/2	29 821.40	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		23/2		23/2	29 821.40	.2	337
$C^{12}H_3C^{12}O^{16}Cl^{37}$	362	2, 1, 2← 1, 0, 1	Ground							20 142.4	.2	384
		2, 1, 2← 1, 0, 1	Ground							20 149.3	.2	384
		3, 1, 3← 2, 0, 2	Ground	AE	0		3/2		1/2	26 165.30	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		5/2		3/2	26 169.10	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		9/2		7/2	26 169.10	.2	337
		3, 1, 3← 2, 0, 2	Ground	AE	0		7/2		5/2	26 172.95	.2	337
		3, 3, 0← 3, 2, 1	Ground							29 342.20	.1	384
		3, 3, 0← 3, 2, 1	Ground							29 343.42	.1	384
		3, 3, 0← 3, 2, 1	Ground							29 348.80	.1	384
		3, 3, 0← 3, 2, 1	Ground							29 350.15	.1	384
		4, 0, 4← 3, 1, 3	Ground	A	0		11/2		9/2	27 046.88	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		11/2		9/2	27 046.88	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		5/2		3/2	27 046.88	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		5/2		3/2	27 046.88	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		9/2		7/2	27 492.96	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		7/2		5/2	27 492.96	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		9/2		7/2	27 493.69	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		7/2		5/2	27 493.69	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		11/2		9/2	27 495.40	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		5/2		3/2	27 495.40	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		11/2		9/2	27 496.12	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		5/2		3/2	27 496.12	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		7/2		7/2	25 962.30	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		13/2		13/2	25 964.05	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		9/2		9/2	25 969.00	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		11/2		11/2	25 970.85	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		13/2		13/2	18 695.28	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		11/2		11/2	18 695.28	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		15/2		15/2	18 695.28	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		9/2		9/2	18 695.28	.2	337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Cl^{37}$	362	6, 2, 4← 6, 1, 5	Ground	A	0		13/2		13/2	18 697.87	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		11/2		11/2	18 697.87	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		15/2		15/2	18 697.87	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		9/2		9/2	18 697.87	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		9/2		9/2	24 014.90	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		15/2		15/2	24 015.90	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		11/2		11/2	24 019.20	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		13/2		13/2	24 020.20	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		15/2		15/2	23 172.22	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		13/2		13/2	23 172.22	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		17/2		17/2	23 172.22	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		11/2		11/2	23 172.22	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		15/2		15/2	23 176.50	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		13/2		13/2	23 176.50	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		17/2		17/2	23 176.50	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		11/2		11/2	23 176.50	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		11/2		11/2	22 846.60	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		17/2		17/2	22 847.27	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		11/2		11/2	22 847.27	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		17/2		17/2	22 848.00	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		13/2		13/2	22 849.41	.2	337
		7, 3, 4← 7, 2, 5	Ground	E	0		15/2		15/2	22 850.10	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		13/2		13/2	22 850.10	.2	337
		7, 3, 4← 7, 2, 5	Ground	A	0		15/2		15/2	22 850.83	.2	337
		8, 2, 6← 8, 1, 7	Ground	E	0		17/2		17/2	29 342.20	.2	337
		8, 2, 6← 8, 1, 7	Ground	E	0		15/2		15/2	29 342.20	.2	337
		8, 2, 6← 8, 1, 7	Ground	A	0		19/2		19/2	29 343.42	.2	337
		8, 2, 6← 8, 1, 7	Ground	A	0		13/2		13/2	29 343.42	.2	337
		8, 2, 6← 8, 1, 7	Ground	E	0		17/2		17/2	29 348.80	.2	337
		8, 2, 6← 8, 1, 7	Ground	E	0		15/2		15/2	29 348.80	.2	337
		8, 2, 6← 8, 1, 7	Ground	A	0		19/2		19/2	29 350.15	.2	337
		8, 2, 6← 8, 1, 7	Ground	A	0		13/2		13/2	29 350.15	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		13/2		13/2	23 120.90	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		19/2		19/2	23 120.90	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		15/2		15/2	23 120.90	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		17/2		17/2	23 120.90	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		13/2		13/2	23 122.25	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		19/2		19/2	23 122.25	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		15/2		15/2	23 122.25	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		17/2		17/2	23 122.25	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		19/2		19/2	25 279.18	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		17/2		17/2	25 279.18	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		21/2		21/2	25 279.18	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		15/2		15/2	25 279.18	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		19/2		19/2	25 282.92	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		17/2		17/2	25 282.92	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		21/2		21/2	25 282.92	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		15/2		15/2	25 282.92	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		21/2		21/2	29 521.30	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		19/2		19/2	29 521.30	.2	337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}Cl^{37}$	362	10, 3, 7←10, 2, 8	Ground	E	0		23/2		23/2	29 522.04	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		17/2		17/2	29 522.04	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		21/2		21/2	29 527.40	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		19/2		19/2	29 527.40	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		23/2		23/2	29 528.13	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		17/2		17/2	29 528.13	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		19/2		19/2	20 067.30	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		25/2		25/2	20 067.30	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		23/2		23/2	29 821.40	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		21/2		21/2	29 821.40	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		21/2		21/2	30 068.48	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		23/2		23/2	30 068.48	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		19/2		19/2	30 069.05	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		25/2		25/2	30 069.05	.2	337
$C^{12}D_3C^{12}O^{16}Cl^{35}$	363	2, 1, 2← 1, 0, 1	Ground	AE	0		1/2		1/2	18 048.30		337
		2, 1, 2← 1, 0, 1	Ground	AE	0		5/2		5/2	18 049.90		337
		2, 1, 2← 1, 0, 1	Ground	AE	0		7/2		5/2	18 055.36		337
		2, 1, 2← 1, 0, 1	Ground	AE	0		5/2		3/2	18 062.50		337
		3, 0, 3← 2, 1, 2	Ground							18 644.05	.1	384
		3, 0, 3← 2, 1, 2	Ground							18 648.50	.1	384
		3, 0, 3← 2, 1, 2	Ground							18 650.70	.1	384
		3, 1, 3← 2, 0, 2	Ground	AE	0		3/2		1/2	23 662.10		337
		3, 1, 3← 2, 0, 2	Ground	AE	0		5/2		3/2	23 666.35		337
		3, 1, 3← 2, 0, 2	Ground	AE	0		9/2		7/2	23 667.22		337
		3, 1, 3← 2, 0, 2	Ground	AE	0		7/2		5/2	23 671.50		337
		3, 1, 3← 2, 0, 2	Ground	AE	0		3/2		3/2	23 674.50		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		7/2		5/2	26 125.90		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		9/2		7/2	26 125.90		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		5/2		3/2	26 128.35		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		11/2		9/2	26 128.35		337
		4, 1, 4← 3, 0, 3	Ground	AE	0		5/2		3/2	29 066.43		337
		4, 1, 4← 3, 0, 3	Ground	AE	0		7/2		5/2	29 068.51		337
		4, 1, 4← 3, 0, 3	Ground	AE	0		11/2		9/2	29 068.51		337
		4, 1, 4← 3, 0, 3	Ground	AE	0		9/2		7/2	29 070.50		337
		4, 1, 4← 3, 0, 3	Ground	AE	0		7/2		7/2	29 074.00		337
		4, 2, 3← 4, 1, 4	Ground	AE	0		11/2		11/2	22 441.05		337
		4, 2, 3← 4, 1, 4	Ground	AE	0		5/2		5/2	22 441.05		337
		4, 2, 3← 4, 1, 4	Ground	AE	0		7/2		7/2	22 444.25		337
		4, 2, 3← 4, 1, 4	Ground	AE	0		9/2		9/2	22 444.25		337
		5, 3, 2← 5, 2, 3	Ground	AE	0		7/2		7/2	20 171.82		337
		5, 3, 2← 5, 2, 3	Ground	AE	0		13/2		13/2	20 173.96		337
		5, 3, 2← 5, 2, 3	Ground	AE	0		9/2		9/2	20 179.30		337
		5, 3, 2← 5, 2, 3	Ground	AE	0		11/2		11/2	20 181.40		337
		5, 3, 2← 5, 2, 3	Ground							20 183.80	.1	384
		5, 3, 3← 5, 2, 4	Ground	AE	0		7/2		7/2	27 010.3		337
		5, 3, 3← 5, 2, 4	Ground	AE	0		13/2		13/2	27 011.9		337
		5, 3, 3← 5, 2, 4	Ground	AE	0		9/2		9/2	27 016.2		337
		5, 3, 3← 5, 2, 4	Ground	AE	0		11/2		11/2	27 017.7		337
		6, 3, 3← 6, 2, 4	Ground	AE	0		9/2		9/2	18 724.40		337
		6, 3, 3← 6, 2, 4	Ground	AE	0		15/2		15/2	18 724.40		337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3C^{12}O^{16}Cl^{35}$	363	6, 3, 3← 6, 2, 4	Ground	AE	0		11/2		11/2	18 725.55		337
		6, 3, 3← 6, 2, 4	Ground	AE	0		13/2		13/2	18 725.55		337
		7, 2, 5← 7, 1, 6	Ground	AE	0		11/2		11/2	22 027.80		337
		7, 2, 5← 7, 1, 6	Ground	AE	0		17/2		17/2	22 027.80		337
		7, 2, 5← 7, 1, 6	Ground	AE	0		13/2		13/2	22 028.93		337
		7, 2, 5← 7, 1, 6	Ground	AE	0		15/2		15/2	22 028.93		337
		7, 3, 4← 7, 2, 5	Ground	AE	0		11/2		11/2	18 427.00		337
		7, 3, 4← 7, 2, 5	Ground	AE	0		17/2		17/2	18 427.00		337
		7, 3, 4← 7, 2, 5	Ground	AE	0		13/2		13/2	18 429.23		337
		7, 3, 4← 7, 2, 5	Ground	AE	0		15/2		15/2	18 429.23		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		13/2		13/2	19 836.38		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		19/2		19/2	19 836.38		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		15/2		15/2	19 837.06		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		17/2		17/2	19 837.06		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		19/2		19/2	23 242.90		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		17/2		17/2	23 242.90		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		21/2		21/2	23 242.90		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		15/2		15/2	23 242.90		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		15/2		15/2	24 862.10		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		21/2		21/2	24 862.10		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		17/2		17/2	24 865.15		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		19/2		19/2	24 865.15		337
		10, 4, 6←10, 3, 7	Ground	AE	0		17/2		17/2	24 235.00		337
		10, 4, 6←10, 3, 7	Ground	AE	0		23/2		23/2	24 235.00		337
		10, 4, 6←10, 3, 7	Ground	AE	0		19/2		19/2	24 236.35		337
		10, 4, 6←10, 3, 7	Ground	AE	0		21/2		21/2	24 236.35		337
		11, 4, 7←11, 3, 8	Ground	AE	0		19/2		19/2	25 585.28		337
		11, 4, 7←11, 3, 8	Ground	AE	0		25/2		25/2	25 585.28		337
		11, 4, 7←11, 3, 8	Ground	AE	0		21/2		21/2	25 585.28		337
		11, 4, 7←11, 3, 8	Ground	AE	0		23/2		23/2	25 585.28		337
$C^{12}D_3C^{12}O^{16}Cl^{37}$	364	3, 1, 3← 2, 0, 2	Ground	AE	0		9/2		7/2	23 382.73		337
		3, 1, 3← 2, 0, 2	Ground	AE	0		7/2		5/2	23 386.40		337
		3, 1, 3← 2, 0, 2	Ground	AE	0		3/2		3/2	23 388.60		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		7/2		5/2	25 441.10		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		9/2		7/2	25 441.10		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		5/2		3/2	25 443.15		337
		4, 0, 4← 3, 1, 3	Ground	AE	0		11/2		9/2	25 443.15		337
		4, 1, 4← 3, 0, 3	Ground							28 662.85	.1	384
		4, 1, 4← 3, 0, 3	Ground							28 664.17	.1	384
		4, 1, 4← 3, 0, 3	Ground	AE	0		11/2		9/2	28 667.02		337
		4, 1, 4← 3, 0, 3	Ground	AE	0		7/2		5/2	28 667.02		337
		4, 1, 4← 3, 0, 3	Ground	AE	0		9/2		7/2	28 668.73		337
		5, 0, 5← 4, 1, 4	Ground							32 346.0	.2	384
		6, 3, 4← 6, 2, 5	Ground							29 179.00	.1	384
		7, 2, 5← 7, 1, 6	Ground	AE	0		11/2		11/2	21 123.0		337
		7, 2, 5← 7, 1, 6	Ground	AE	0		17/2		17/2	21 123.0		337
		7, 2, 5← 7, 1, 6	Ground	AE	0		15/2		15/2	21 123.0		337
		7, 2, 5← 7, 1, 6	Ground	AE	0		13/2		13/2	21 123.0		337
		7, 3, 4← 7, 2, 5	Ground	AE	0		17/2		17/2	18 730.03		337
		7, 3, 4← 7, 2, 5	Ground	AE	0		11/2		11/2	18 730.03		337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3C^{12}O^{16}Cl^{37}$	364	7, 3, 4← 7, 2, 5	Ground	AE	0		15/2		15/2	18 732.27		337
		7, 3, 4← 7, 2, 5	Ground	AE	0		13/2		13/2	18 732.27		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		13/2		13/2	19 667.25		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		19/2		19/2	19 667.25		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		17/2		17/2	19 667.25		337
		8, 3, 5← 8, 2, 6	Ground	AE	0		15/2		15/2	19 667.25		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		19/2		19/2	22 470.92		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		21/2		21/2	22 470.92		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		17/2		17/2	22 470.92		337
		9, 3, 6← 9, 2, 7	Ground	AE	0		15/2		15/2	22 470.92		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		21/2		21/2	25 827.40		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		15/2		15/2	25 827.40		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		17/2		17/2	25 829.70		337
		9, 4, 5← 9, 3, 6	Ground	AE	0		19/2		19/2	25 829.70		337
		10, 4, 6←10, 3, 7	Ground	AE	0		23/2		23/2	24 725.0		337
		10, 4, 6←10, 3, 7	Ground	AE	0		17/2		17/2	24 725.0		337
		10, 4, 6←10, 3, 7	Ground	AE	0		19/2		19/2	24 725.0		337
		10, 4, 6←10, 3, 7	Ground	AE	0		21/2		21/2	24 725.0		337
		11, 4, 7←11, 3, 8	Ground	AE	0		19/2		19/2	25 356.28		337
		11, 4, 7←11, 3, 8	Ground	AE	0		25/2		25/2	25 356.28		337
		11, 4, 7←11, 3, 8	Ground	AE	0		23/2		23/2	25 357.04		337
		11, 4, 7←11, 3, 8	Ground	AE	0		21/2		21/2	25 357.04		337
		12, 4, 8←12, 3, 9	Ground							28 139.55	.1	384
		12, 4, 8←12, 3, 9	Ground							28 141.00	.1	384
s-$C^{12}H_2DC^{12}O^{16}Cl^{35}$	365	3, 0, 3← 2, 1, 2	Ground							18 758.5	.2	337
		3, 0, 3← 2, 1, 2	Ground							18 759.0	.2	384
		3, 1, 3← 2, 0, 2	Ground							25 623.0	.2	337
		4, 0, 4← 3, 1, 3	Ground							26 821.50	.1	384
		4, 0, 4← 3, 1, 3	Ground							26 822.75	.2	337
		4, 0, 4← 3, 1, 3	Ground							26 824.00	.1	384
		5, 1, 4← 5, 0, 5	Ground							21 695.4	.2	384
		5, 1, 4← 5, 0, 5	Ground							21 697.58	.2	337 [1]
		5, 1, 4← 5, 0, 5	Ground							21 698.15	.1	384
		5, 1, 4← 5, 0, 5	Ground							21 699.75	.1	384
		5, 3, 2← 5, 2, 3	Ground							25 655.5	.2	384
		5, 3, 2← 5, 2, 3	Ground							25 657.85	.2	337
		6, 2, 4← 6, 1, 5	Ground							18 275.45	.2	337
		6, 3, 3← 6, 2, 4	Ground							23 737.50	.2	337
		7, 2, 5← 7, 1, 6	Ground							22 573.05	.1	384
		7, 2, 5← 7, 1, 6	Ground							22 574.10	.1	384
		7, 2, 5← 7, 1, 6	Ground							25 573.58	.2	337
		7, 3, 4← 7, 2, 5	Ground							22 544.60	.1	384
		7, 3, 4← 7, 2, 5	Ground							22 546.25	.2	337
		7, 3, 4← 7, 2, 5	Ground							22 547.90	.1	384
		8, 2, 6← 8, 1, 7	Ground							28 513.80	.1	384
		8, 2, 6← 8, 1, 7	Ground							28 514.05	.2	337
		8, 3, 5← 8, 2, 6	Ground							22 726.75	.1	384
		8, 3, 5← 8, 2, 6	Ground							22 727.54	.2	337
		8, 3, 5← 8, 2, 6	Ground							22 728.32	.1	384
		9, 3, 6← 9, 2, 7	Ground							24 722.25	.2	337

1. The transition in Sinnott's article listed as 5_{15}←5_{05} is forbidden and assumed to have been a misprint. It has been entered as 5_{14}←5_{05}, an allowable "b" transition.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
s-$C^{12}H_2DC^{12}O^{16}Cl^{35}$	365	10, 3, 7←10, 2, 8	Ground							28 739.25	.2	337
a-$C^{12}H_2DC^{12}O^{16}Cl^{35}$	366	2, 1, 2← 1, 0, 1	Ground							19 352.5	.2	384
		4, 0, 4← 3, 1, 3	Ground							27 896.28	.1	384
		4, 0, 4← 3, 1, 3	Ground							27 897.37	.2	337
		4, 0, 4← 3, 1, 3	Ground							27 898.46	.1	384
		4, 1, 4← 3, 0, 3	Ground							31 064.53	.1	384
		4, 1, 4← 3, 0, 3	Ground							31 065.70	.2	337
		4, 1, 4← 3, 0, 3	Ground							31 066.86	.1	384
		5, 1, 4← 5, 0, 5	Ground							22 782.10	.1	384
		5, 1, 4← 5, 0, 5	Ground							22 784.10	.2	337
		5, 1, 4← 5, 0, 5	Ground							22 786.10	.1	384
		5, 3, 2← 5, 2, 3	Ground							21 840.5	.2	384
		5, 3, 2← 5, 2, 3	Ground							21 844.75	.2	337
		6, 2, 4← 6, 1, 5	Ground							18 577.95	.2	337
		6, 2, 4← 6, 1, 5	Ground							18 578.3	.2	384
		7, 2, 5← 7, 1, 6	Ground							24 015.28	.2	337
		7, 3, 4← 7, 2, 5	Ground							19 987.2	.2	384
		7, 3, 4← 7, 2, 5	Ground							19 988.0	.2	337
		8, 3, 5← 8, 2, 6	Ground							21 565.5	.2	337
		9, 3, 6← 9, 2, 7	Ground							25 324.9	.2	337
		9, 4, 5← 9, 3, 6	Ground							26 909.85	.1	384
		9, 4, 5← 9, 3, 6	Ground							26 911.43	.2	337
		9, 4, 5← 9, 3, 6	Ground							26 913.00	.1	384
		10, 3, 7←10, 2, 8	Ground							31 193.77	.1	384
		10, 3, 7←10, 2, 8	Ground							31 195.35	.1	384
		10, 3, 7←10, 2, 8	Ground							31 196.34	.1	384
		10, 3, 7←10, 2, 8	Ground							31 197.88	.1	384
		10, 4, 6←10, 3, 7	Ground							26 281.5	.2	337
		10, 4, 6←10, 3, 7	Ground							26 282.0	.2	384
$C^{13}H_3C^{12}O^{16}Cl^{35}$	367	4, 0, 4← 3, 1, 3	Ground	E	0		9/2		7/2	27 813.90	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		7/2		5/2	27 813.90	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		9/2		7/2	27 813.90	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		7/2		5/2	27 813.90	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		11/2		9/2	27 816.80	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		5/2		3/2	27 816.80	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		11/2		9/2	27 816.80	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		5/2		3/2	27 816.80	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		7/2		7/2	24 179.60	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		13/2		13/2	24 181.90	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		9/2		9/2	24 188.08	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		11/2		11/2	24 190.08	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		13/2		13/2	18 816.30	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		11/2		11/2	18 816.30	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		15/2		15/2	18 816.30	.2	337
		6, 2, 4← 6, 1, 5	Ground	E	0		9/2		9/2	18 816.30	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		13/2		13/2	18 819.38	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		11/2		11/2	18 819.38	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		15/2		15/2	18 819.38	.2	337
		6, 2, 4← 6, 1, 5	Ground	A	0		9/2		9/2	18 819.38	.2	337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_3C^{12}O^{16}Cl^{35}$	367	6, 3, 3← 6, 2, 4	Ground	AE	0		9/2		9/2	22 371.19	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		15/2		15/2	22 371.19	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		11/2		11/2	22 376.50	.2	337
		6, 3, 3← 6, 2, 4	Ground	AE	0		13/2		13/2	22 376.50	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		15/2		15/2	23 841.25	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		13/2		13/2	23 841.25	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		17/2		17/2	23 842.59	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		11/2		11/2	23 842.59	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		15/2		15/2	23 846.17	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		13/2		13/2	23 846.17	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		17/2		17/2	23 847.47	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		11/2		11/2	23 847.47	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		13/2		13/2	22 491.47	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		19/2		19/2	22 491.47	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		15/2		15/2	22 492.59	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		17/2		17/2	22 492.59	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		13/2		13/2	22 493.90	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		19/2		19/2	22 493.90	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		15/2		15/2	22 495.00	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		17/2		17/2	22 495.00	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		19/2		19/2	25 466.03	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		17/2		17/2	25 466.03	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		21/2		21/2	25 466.03	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		15/2		15/2	25 466.03	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		19/2		19/2	25 470.35	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		17/2		17/2	25 470.35	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		21/2		21/2	25 470.35	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		15/2		15/2	25 470.35	.2	337
$C^{13}H_3C^{12}O^{16}Cl^{37}$	368	4, 0, 4← 3, 1, 3	Ground	E	0		9/2		7/2	27 044.25	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		7/2		5/2	27 044.25	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		9/2		7/2	27 044.25	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		7/2		5/2	27 044.25	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		15/2		15/2	22 908.0	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		13/2		13/2	22 908.0	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		17/2		17/2	22 908.0	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		11/2		11/2	22 908.0	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		15/2		15/2	22 912.1	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		13/2		13/2	22 912.1	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		17/2		17/2	22 912.1	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		11/2		11/2	22 912.1	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		19/2		19/2	24 822.00	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		17/2		17/2	24 822.00	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		21/2		21/2	24 822.00	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		15/2		15/2	24 822.00	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		19/2		19/2	24 825.58	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		17/2		17/2	24 825.58	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		21/2		21/2	24 825.58	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		15/2		15/2	24 825.58	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		21/2		21/2	29 932.42	.2	337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_3C^{12}O^{16}Cl^{37}$	368	10, 3, 7←10, 2, 8	Ground	E	0		19/2		19/2	29 932.42	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		23/2		23/2	29 932.42	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		17/2		17/2	29 932.42	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		23/2		23/2	29 938.48	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		21/2		21/2	29 938.48	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		19/2		19/2	29 938.48	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		17/2		17/2	29 938.48	.2	337
$C^{12}H_3C^{13}O^{16}Cl^{35}$	369	4, 0, 4← 3, 1, 3	Ground	E	0		9/2		7/2	28 196.8	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		7/2		5/2	28 196.8	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		9/2		7/2	28 196.8	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		7/2		5/2	28 196.8	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		11/2		9/2	28 199.6	.2	337
		4, 0, 4← 3, 1, 3	Ground	E	0		5/2		3/2	28 199.6	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		11/2		9/2	28 199.6	.2	337
		4, 0, 4← 3, 1, 3	Ground	A	0		5/2		3/2	28 199.6	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		7/2		7/2	25 223.87	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		13/2		13/2	25 227.20	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		9/2		9/2	25 230.51	.2	337
		5, 3, 2← 5, 2, 3	Ground	AE	0		11/2		11/2	25 232.97	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		15/2		15/2	23 989.95	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		13/2		13/2	23 989.95	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		17/2		17/2	23 991.05	.2	337
		7, 2, 5← 7, 1, 6	Ground	E	0		11/2		11/2	23 991.05	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		15/2		15/2	23 995.15	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		13/2		13/2	23 995.15	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		17/2		17/2	23 996.28	.2	337
		7, 2, 5← 7, 1, 6	Ground	A	0		11/2		11/2	23 996.28	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		13/2		13/2	23 066.35	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		19/2		19/2	23 066.35	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		15/2		15/2	23 067.67	.2	337
		8, 3, 5← 8, 2, 6	Ground	E	0		17/2		17/2	23 067.67	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		13/2		13/2	23 068.63	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		19/2		19/2	23 068.63	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		15/2		15/2	23 069.90	.2	337
		8, 3, 5← 8, 2, 6	Ground	A	0		17/2		17/2	23 069.90	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		19/2		19/2	25 791.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		17/2		17/2	25 791.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		21/2		21/2	25 791.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		15/2		15/2	25 791.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		19/2		19/2	25 796.17	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		17/2		17/2	25 796.17	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		21/2		21/2	25 796.17	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		15/2		15/2	25 796.17	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		21/2		21/2	30 696.01	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		19/2		19/2	30 696.01	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		23/2		23/2	30 697.15	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		17/2		17/2	30 697.15	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		21/2		21/2	30 702.86	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		19/2		19/2	30 702.86	.2	337

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{13}O^{16}Cl^{35}$	369	10, 3, 7←10, 2, 8	Ground	A	0		23/2		23/2	30 703.99	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		17/2		17/2	30 703.99	.2	337
$C^{12}H_3C^{13}O^{16}Cl^{37}$	371	10, 3, 7←10, 2, 8	Ground	E	0		21/2		21/2	29 390.91	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		19/2		19/2	29 390.91	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		23/2		23/2	29 390.91	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		17/2		17/2	29 390.91	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		21/2		21/2	29 396.97	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		19/2		19/2	29 396.97	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		23/2		23/2	29 396.97	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		17/2		17/2	29 396.97	.2	337
$C^{12}H_3C^{12}O^{18}Cl^{35}$	372	9, 3, 6← 9, 2, 7	Ground	E	0		19/2		19/2	25 411.05	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		19/2		19/2	25 414.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		17/2		17/2	25 414.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		21/2		21/2	25 414.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	A	0		15/2		15/2	25 414.85	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		21/2		21/2	25 441.05	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		15/2		15/2	25 441.05	.2	337
		9, 3, 6← 9, 2, 7	Ground	E	0		17/2		17/2	25 441.05	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		21/2		21/2	30 988.90	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		19/2		19/2	30 988.90	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		23/2		23/2	30 988.90	.2	337
		10, 3, 7←10, 2, 8	Ground	E	0		17/2		17/2	30 988.90	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		21/2		21/2	30 995.70	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		19/2		19/2	30 995.70	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		23/2		23/2	30 995.70	.2	337
		10, 3, 7←10, 2, 8	Ground	A	0		17/2		17/2	30 995.70	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		19/2		19/2	28 338.33	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		25/2		25/2	28 338.33	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		21/2		21/2	28 338.33	.2	337
		11, 4, 7←11, 3, 8	Ground	E	0		23/2		23/2	28 338.33	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		19/2		19/2	28 341.10	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		25/2		25/2	28 341.10	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		21/2		21/2	28 341.10	.2	337
		11, 4, 7←11, 3, 8	Ground	A	0		23/2		23/2	28 341.10	.2	337
		12, 4, 8←12, 3, 9	Ground	E	0		21/2		21/2	31 811.40	.2	337
		12, 4, 8←12, 3, 9	Ground	E	0		27/2		27/2	31 811.40	.2	337
		12, 4, 8←12, 3, 9	Ground	E	0		23/2		23/2	31 811.40	.2	337
		12, 4, 8←12, 3, 9	Ground	E	0		25/2		25/2	31 811.40	.2	337
		12, 4, 8←12, 3, 9	Ground	A	0		21/2		21/2	31 817.55	.2	337
		12, 4, 8←12, 3, 9	Ground	A	0		27/2		27/2	31 817.55	.2	337
		12, 4, 8←12, 3, 9	Ground	A	0		23/2		23/2	31 817.55	.2	337
		12, 4, 8←12, 3, 9	Ground	A	0		25/2		25/2	31 817.55	.2	337

$C_2H_3Cl_3$ $C_{3v}(C_{3v},C_{3v})$ CH_3CCl_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}Cl_3^{35}$	C_{3v}	381	2 372.6 M	2 372.6 M					

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
381	0. X	0. X	1.79 G		3000						

1. Assumed CCl_3 configuration as in chloroform and CH_3 as in methane.

References:

ABC: 53 D_J: D_{JK}: κ: Δ:

μ: 388 eQq: V: 113 I: ω:

Add. Ref.: 160

1,1,1-Trichloroethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}Cl_3^{35}$	381	5, ← 4, 8, ← 7,	Ground Ground						23 735. 37 955.88	10. .40	158 53

C_2H_3FO $C_s(C_{3v},C_s)$ CH_3COF

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}O^{16}F^{19}$	C_s	391	11 039.28 M	9 685.65 M	5 322.05 M				3.000
$C^{12}D_3C^{12}O^{16}F^{19}$	C_s	392	10 319.46 M	7 986.06 M	4 763.02 M				6.153
$C^{13}H_3C^{12}O^{16}F^{19}$	C_s	393	11 038.83 M	9 309.72 M	5 206.44 M				
$C^{12}H_3C^{12}O^{18}F^{19}$	C_s	394	10 522.74 M	9 470.63 M	5 136.20 M				
s-$C^{12}HD_2C^{12}O^{16}F^{19}$	C_s	395	10 586.16 M	8 420.42 M	4 971.86 M				6.112
a-$C^{12}HD_2C^{12}O^{16}F^{19}$	C_1	396	10 591.19 M	8 467.89 M	4 908.64 M				
s-$C^{12}H_2DC^{12}O^{16}F^{19}$	C_s	397	10 919.20 M	8 971.39 M	5 075.09 M				3.036
a-$C^{12}H_2DC^{12}O^{16}F^{19}$	C_1	398	10 805.96 M	9 016.47 M	5 134.54 M				
$C^{12}H_3C^{13}O^{16}F^{19}$	C_s	399	11 034.56 M	9 686.60 M	5 321.32 M				
$C^{12}D_3C^{13}O^{16}F^{19}$	C_s	401	10 315.05 M	7 985.33 M	4 761.80 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
391	2.83 M	0.88 M	0. X		1041	6					
392					1031	6					
394	2.92 M	0.30 M	0. X		1055	6					

References:

ABC: 263 D_J: D_{JK}: κ: Δ: 263

μ: 263 eQq: V: 263 I: ω:

Add. Ref.: 150

For species 391, 392, 393, and 394, the coupling parameter is $I_\alpha = 3.158$ amu Å^2. Ref: 263.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}F^{19}$	391	1, 0, 1← 0, 0, 0	Ground	A	0					15 007.91	.2	263
		2, 0, 2← 1, 0, 1	Ground	E	0					26 734.61	.2	263
		2, 0, 2← 1, 0, 1	Ground	A	0					26 739.20	.2	263
		2, 1, 1← 1, 1, 0	Ground	A	0					34 379.40	.2	263
		2, 1, 2← 1, 1, 1	Ground	A	0					25 651.87	.2	263
		2, 1, 1← 2, 1, 2	Ground							13 091.42	.2	261
		3, 0, 3← 2, 0, 2	Ground	E	0					37 051.64	.2	263
		3, 0, 3← 2, 0, 2	Ground	A	0					37 055.85	.2	263
		3, 1, 2← 3, 1, 3	Ground	E	0					24 072.41	.2	263
		3, 1, 2← 3, 1, 3	Ground	A	0					24 079.83	.2	263
		4, 2, 2← 4, 2, 3	Ground	A	0					22 512.80	.2	263
		4, 2, 2← 4, 2, 3	Ground	E	0					22 518.13	.2	263
		5, 3, 2← 5, 3, 3	Ground	A	0					20 073.25	.2	263
		5, 3, 2← 5, 3, 3	Ground	E	0					20 094.58	.2	263
		6, 4, 2← 6, 4, 3	Ground	A	0					16 935.00	.2	263
		6, 4, 2← 6, 4, 3	Ground	E	0					16 972.60	.2	263
		8, 5, 3← 8, 5, 4	Ground	A	0					26 679.20	.2	263
		8, 5, 3← 8, 5, 4	Ground	E	0					26 732.94	.2	263
		9, 6, 3← 9, 6, 4	Ground	A	0					22 427.90	.2	263
		9, 6, 3← 9, 6, 4	Ground	E	0					22 505.64	.2	263
		10, 7, 3←10, 7, 4	Ground	A	0					17 745.20	.2	263
		10, 7, 3←10, 7, 4	Ground	E	0					17 839.23	.2	263
		Not Reported	Ground							15 802.28	.2	261
		Not Reported	Ground							15 886.51	.2	261
		Not Reported	Ground							15 938.33	.2	261
		Not Reported	Ground							16 205.5	.2	261
		Not Reported	Ground							16 243.4	.2	261
		Not Reported	Ground							16 273.5	.2	261
		Not Reported	Ground							16 285.8	.2	261
		Not Reported	Ground							16 314.8	.2	261
		Not Reported	Ground							20 095.87	.2	261
		Not Reported	Ground							22 514.20	.2	261
		Not Reported	Ground							22 556.28	.2	261
		Not Reported	Ground							23 470.99	.2	261
		Not Reported	Ground							23 487.11	.2	261
		Not Reported	Ground							24 017.14	.2	261
		Not Reported	Ground							24 138.78	.2	261
		Not Reported	Ground							25 186.63	.2	261
		Not Reported	Ground							25 279.90	.2	261
		Not Reported	Ground							25 354.51	.2	261
		Not Reported	Ground							25 382.23	.2	261
		Not Reported	Ground							25 403.68	.2	261
		Not Reported	Ground							25 408.60	.2	261
		Not Reported	Ground							25 413.40	.2	261
		Not Reported	Ground							25 437.8	.2	261
		Not Reported	Ground							25 619.50	.2	261
		Not Reported	Ground							25 658.53	.2	261
		Not Reported	Ground							26 144.27	.2	261
		Not Reported	Ground							26 239.61	.2	261
		Not Reported	Ground							26 612.3	.2	261

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}F^{19}$	391	Not Reported	Ground							26 668.7	.2	261
		Not Reported	Ground							26 723.74	.2	261
$C^{12}D_3C^{12}O^{16}F^{19}$	392	2, 0, 2← 1, 0, 1	Ground	A	0					23 722.63	.2	263
		2, 1, 1← 1, 1, 0	Ground	A	0					28 721.12	.2	263
		2, 1, 2← 1, 1, 1	Ground	A	0					22 275.12	.2	263
		3, 1, 3← 3, 1, 2	Ground	A	0					18 608.04	.2	263
		4, 1, 3← 4, 1, 4	Ground	A	0					28 226.45	.2	263
		4, 2, 2← 4, 2, 3	Ground	A	0					15 186.50	.2	263
		5, 2, 3← 5, 2, 4	Ground	A	0					25 426.89	.2	263
		6, 3, 3← 6, 3, 4	Ground	A	0					20 948.04	.2	263
		7, 4, 3← 7, 4, 4	Ground	A	0					15 438.90	.2	263
		7, 4, 3← 7, 4, 4	Ground	E	0					15 440.93	.2	263
		8, 4, 4← 8, 4, 5	Ground	A	0					26 977.99	.2	263
		8, 4, 4← 8, 4, 5	Ground	E	0					26 980.24	.2	263
		9, 5, 4← 9, 5, 5	Ground	A	0					20 356.01	.2	263
		9, 5, 4← 9, 5, 5	Ground	E	0					20 359.26	.2	263
		10, 6, 4←10, 6, 5	Ground	A	0					13 528.40	.2	263
		10, 6, 4←10, 6, 5	Ground	E	0					13 531.55	.2	263
		11, 6, 5←11, 6, 6	Ground	A	0					25 680.09	.2	263
		11, 6, 5←11, 6, 6	Ground	E	0					25 684.02	.2	263
		12, 7, 5←12, 7, 6	Ground	A	0					17 650.87	.2	263
		12, 7, 5←12, 7, 6	Ground	E	0					17 655.53	.2	263
		Not Reported	Ground							20 898.95	.2	261
		Not Reported	Ground							23 861.4	.2	261
$C^{13}H_3C^{12}O^{16}F^{19}$	393	2, 0, 2← 1, 0, 1	Ground	E	0					26 214.86	.2	263
		2, 0, 2← 1, 0, 1	Ground	A	0					26 218.70	.2	263
		2, 1, 1← 1, 1, 0	Ground	A	0					33 135.80	.2	263
		2, 1, 2← 1, 1, 1	Ground	A	0					24 929.38	.2	263
		3, 1, 2← 3, 1, 3	Ground	A	0					23 045.70	.2	263
		3, 1, 2← 3, 1, 3	Ground	E	0					23 050.60	.2	263
		4, 2, 2← 4, 2, 3	Ground	A	0					20 768.85	.2	263
		4, 2, 2← 4, 2, 3	Ground	E	0					20 776.98	.2	263
		6, 3, 3← 6, 3, 4	Ground	A	0					29 965.25	.2	263
		6, 3, 3← 6, 3, 4	Ground	E	0					29 979.27	.2	263
		7, 4, 3← 7, 4, 4	Ground	A	0					26 192.50	.2	263
		7, 4, 3← 7, 4, 4	Ground	E	0					26 228.50	.2	263
		8, 5, 3← 8, 5, 4	Ground	A	0					21 405.82	.2	263
		8, 5, 3← 8, 5, 4	Ground	E	0					21 462.35	.2	263
		10, 6, 4←10, 6, 5	Ground	A	0					30 501.80	.2	263
		10, 6, 4←10, 6, 5	Ground	E	0					30 577.20	.2	263
		11, 7, 4←11, 7, 5	Ground	A	0					24 337.70	.2	263
		11, 7, 4←11, 7, 5	Ground	E	0					24 435.85	.2	263
		12, 8, 4←12, 8, 5	Ground	A	0					17 915.80	.2	263
		12, 8, 4←12, 8, 5	Ground	E	0					18 024.90	.2	263
$C^{12}H_3C^{12}O^{18}F^{19}$	394	1, 1, 1← 0, 0, 0	Ground	A	0					14 606.97	.2	263
		2, 0, 2← 1, 0, 1	Ground	E	0					25 760.73	.2	263
		2, 0, 2← 1, 0, 1	Ground	A	0					25 764.98	.2	263
		2, 1, 1← 1, 1, 1	Ground	A	0					33 547.57	.2	263
		2, 1, 2← 1, 1, 1	Ground	A	0					24 879.75	.2	263

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{18}F^{19}$	394	4, 2, 2← 4, 2, 3	Ground	A	0					22 525.39	.2	263
		4, 2, 2← 4, 2, 3	Ground	E	0					22 527.51	.2	263
		5, 3, 2← 5, 3, 3	Ground	A	0					20 772.09	.2	263
		5, 3, 2← 5, 3, 3	Ground	E	0					20 788.44	.2	263
		6, 4, 2← 6, 4, 3	Ground	A	0					18 382.46	.2	263
		6, 4, 2← 6, 4, 3	Ground	E	0					18 414.95	.2	263
		8, 5, 3← 8, 5, 4	Ground	A	0					28 646.37	.2	263
		8, 5, 3← 8, 5, 4	Ground	E	0					28 685.18	.2	263
		9, 6, 3← 9, 6, 4	Ground	A	0					25 563.55	.2	263
		9, 6, 3← 9, 6, 4	Ground	E	0					25 626.39	.2	263
		10, 7, 3←10, 7, 4	Ground	A	0					21 868.34	.2	263
		10, 7, 3←10, 7, 4	Ground	E	0					21 952.95	.2	263
s-$C^{12}HD_2C^{12}O^{16}F^{19}$	395	2, 0, 2← 1, 0, 1	Ground							24 756.10	.2	263
		2, 1, 1← 1, 1, 0	Ground							30 233.13	.2	263
		2, 1, 2← 1, 1, 1	Ground							23 336.00	.2	263
		6, 3, 3← 6, 3, 4	Ground							23 400.00	.2	263
		7, 4, 3← 7, 4, 4	Ground							18 233.5	.2	263
		8, 4, 4← 8, 4, 5	Ground							30 549.9	.2	263
		9, 5, 4← 9, 5, 5	Ground							24 490.4	.2	263
		12, 7, 5←12, 7, 6	Ground							23 513.4	.2	261
a-$C^{12}HD_2C^{12}O^{16}F^{19}$	396	2, 0, 2← 1, 0, 1	Ground							24 612.25	.2	263
		2, 1, 1← 1, 1, 0	Ground							30 312.30	.2	263
		2, 1, 2← 1, 1, 1	Ground							23 193.80	.2	263
		3, 1, 2← 3, 1, 3	Ground							20 356.22	.2	261
		3, 1, 2← 3, 1, 3	Ground							20 359.45	.2	261
		4, 2, 2← 4, 2, 3	Ground							17 319.30	.2	263
		6, 3, 3← 6, 3, 4	Ground							24 460.30	.2	263
		7, 4, 3← 7, 4, 4	Ground							19 412.00	.2	263
		7, 4, 3← 7, 4, 4	Ground							19 413.95	.2	263
		8, 4, 4← 8, 4, 5	Ground							32 052.10	.2	263
		8, 4, 4← 8, 4, 5	Ground							32 054.10	.2	263
		9, 5, 4← 9, 5, 5	Ground							26 193.05	.2	263
		9, 5, 4← 9, 5, 5	Ground							26 196.60	.2	263
		10, 6, 4←10, 6, 5	Ground							19 467.27	.2	263
		10, 6, 4←10, 6, 5	Ground							19 471.22	.2	263
		12, 7, 6←12, 7, 5	Ground							25 912.13	.2	261
		12, 7, 6←12, 7, 5	Ground							25 917.58	.2	261
s-$C^{12}H_2DC^{12}O^{16}F^{19}$	397	2, 0, 2← 1, 0, 1	Ground							25 576.50	.2	263
		2, 1, 1← 1, 1, 0	Ground							31 989.25	.2	263
		2, 1, 2← 1, 1, 1	Ground							24 196.65	.2	263
		7, 4, 3← 7, 4, 4	Ground							23 281.	5.	263
		10, 6, 4←10, 6, 5	Ground							25 519.13	.2	263
a-$C^{12}H_2DC^{12}O^{16}F^{19}$	398	2, 0, 2← 1, 0, 1	Ground							25 719.08	.2	263
		2, 0, 2← 1, 0, 1	Ground							25 720.39	.2	263
		2, 1, 1← 1, 1, 0	Ground							31 283.38	.2	263
		2, 1, 2← 1, 1, 1	Ground							24 420.07	.2	263
		3, 1, 2← 3, 1, 3	Ground							21 907.91	.2	261
		3, 1, 2← 3, 1, 3	Ground							21 909.71	.2	261

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
a-$C^{12}H_2DC^{12}O^{16}F^{19}$	398	4, 1, 3← 4, 1, 4	Ground							32 191.8	.2	261
		4, 2, 2← 4, 2, 3	Ground							19 487.98	.2	263
		4, 2, 2← 4, 2, 3	Ground							19 490.73	.2	263
		5, 2, 3← 5, 2, 4	Ground							30 757.31	.2	261
		5, 2, 3← 5, 2, 4	Ground							30 758.58	.2	261
		5, 3, 2← 5, 3, 3	Ground							16 089.5	.2	261
		5, 3, 2← 5, 3, 3	Ground							16 097.6	.2	261
		6, 3, 3← 6, 3, 4	Ground							28 029.77	.2	263
		6, 3, 3← 6, 3, 4	Ground							28 035.49	.2	263
		7, 4, 3← 7, 4, 4	Ground							23 998.35	.2	263
		7, 4, 3← 7, 4, 4	Ground							24 010.20	.2	263
		8, 4, 4← 8, 4, 5	Ground							19 047.52	.2	263
$C^{12}H_3C^{13}O^{16}F^{19}$	399	2, 1, 2← 1, 1, 1	Ground							25 650.62	.2	263
		3, 1, 2← 3, 1, 3	Ground	E	1					24 082.77	.2	263
		3, 1, 2← 3, 1, 3	Ground	A	1					24 082.84	.2	263
		4, 2, 2← 4, 2, 3	Ground	E	1					22 525.92	.2	263
		4, 2, 2← 4, 2, 3	Ground	A	1					22 526.15	.2	263
		5, 3, 2← 5, 3, 3	Ground	A	1					20 099.10	.2	263
		5, 3, 2← 5, 3, 3	Ground	E	1					20 099.20	.2	263
		9, 6, 3← 9, 6, 4	Ground	E	1					22 506.26	.2	263
		9, 6, 3← 9, 6, 4	Ground	A	1					22 506.98	.2	263
$C^{12}D_3C^{13}O^{16}F^{19}$	401	2, 0, 2← 1, 1, 1	Ground							23 717.18	.2	263
		2, 1, 2← 1, 1, 1	Ground							22 270.72	.2	263
		3, 1, 2← 3, 1, 3	Ground							18 609.24	.2	263
		6, 3, 3← 6, 3, 4	Ground							20 963.63	.2	263
		9, 5, 4← 9, 5, 5	Ground	E	1					20 391.43	.2	263
		9, 5, 4← 9, 5, 5	Ground	A	1					20 391.54	.2	263

$C_2H_3F_3$ $C_{3v}(C_{3v},C_{3v})$ CH_3CF_3

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}F_3^{19}$	C_{3v}	411		5 185.14 M	5 185.14 M	.002	<.005		
$C^{12}H_2DC^{12}F_3^{19}$	C_s	412	5 465.8 M	4 976.41 M	4 947.46 M	.0014			
$C^{12}D_2HC^{12}F_3^{19}$	C_s	413	5 390. M	4 804.78 M	4 743.28 M				
$C^{12}D_3C^{12}F_3^{19}$	C_{3v}	414		4 605.87 M	4 605.87 M				
$C^{13}H_3C^{12}F_3^{19}$	C_{3v}	415		5 060.12 M	5 060.12 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
411	2.27 M	0. X	0. X		3350	120					

References:

ABC: 135, 165, 188, 194 D_J: 135, 188 D_{JK}: 135 κ: Δ:

μ: 370 eQq: V: 51 I: ω:

Add. Refs.: 18, 21, 30

Torsional frequency = 234 ± 40 cm^{-1}. Ref: 43.

1,1,1-Trifluoroethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}F_3^{19}$	411	2, ← 1,	Excited						20 675.2		135
		2, ← 1,	Excited						20 678.2		135
		2, ← 1,	Excited						20 694.8		135
		2, ← 1,	Excited						20 708.18		135
		2, ← 1,	Excited						20 709.7		135
		2, ← 1,	Excited						20 725.0		135
		2, ← 1,	Ground						20 740.53	.1	135
		2, ← 1,	Excited						20 757.4		135
		2, ← 1,	Excited						30 978.5		95
		3, ← 2,	Ground						30 996.5		95
		3, ← 2,	Excited						31 012.82		135
		3, ← 2,	Excited						31 017.20		135
		3, ← 2,	Excited						31 042.2		135
		3, ← 2,	Excited						31 062.06		135
		3, ← 2,	Excited						31 063.97		135
		3, ← 2,	Excited						31 064.68		135
		3, ← 2,	Excited						31 086.8		135
		3, ← 2,	Ground						31 110.67	.1	135
		3, ← 2,	Excited						31 136.0		135
		4, ← 3,	Excited						41 356.06		135
		4, ← 3,	Excited						41 415.94		135
		4, ← 3,	Excited						41 418.30		135
		4, ← 3,	Excited						41 419.48		135
		4, ← 3,	Ground						41 480.72	.1	135
		Not Reported							20 707.4		95

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2DC^{12}F_3^{19}$	412	2, 0, 2← 1, 0, 1	Ground						19 846.45	.2	188
		2, 1, 1← 1, 1, 0	Ground						19 876.68	.2	188
		2, 1, 2← 1, 1, 1	Ground						19 818.74	.2	188
		3, 0, 3← 2, 0, 2	Ground						29 766.45	.2	188
		3, 1, 2← 2, 1, 1	Ground						29 814.08	.2	188
		3, 1, 3← 2, 1, 2	Ground						29 727.20	.2	188
		3, 2, 1← 2, 2, 0	Ground						29 776.39	.2	188
		3, 2, 2← 2, 2, 1	Ground						29 771.66	.2	188
		5, 0, 5← 4, 0, 4	Ground						49 594.30	.2	188
		5, 1, 4← 4, 1, 3	Ground						49 685.20	.2	188
		5, 1, 5← 4, 1, 4	Ground						49 541.22	.2	188
		5, 2, 3← 4, 2, 2	Ground						49 640.22	.2	188
		5, 2, 4← 4, 2, 3	Ground						49 616.02	.2	188
		5, 3, 2← 4, 3, 1	Ground						49 623.16	.2	188
		5, 3, 3← 4, 3, 2	Ground						49 623.16	.2	188
		5, 4, 1← 4, 4, 0	Ground						49 621.46	.2	188
		5, 4, 2← 4, 4, 1	Ground						49 621.46	.2	188
		Not Reported	Ground						29 695.6		165
$C^{12}D_2HC^{12}F_3^{19}$	413	2, 0, 2← 1, 0, 1	Ground						19 090.0	.2	165
		2, 1, 1← 1, 1, 0	Ground						19 157.8	.2	165
		2, 1, 1← 1, 1, 0	Ground						28 519.5	.2	165
		2, 1, 2← 1, 1, 1	Ground						19 034.7	.2	165
		3, 0, 3← 2, 0, 2	Ground						28 625.8	.2	165
		3, 1, 2← 2, 1, 1	Ground						28 734.7	.2	165
		3, 1, 3← 2, 1, 2	Ground						28 549.1	.2	165
		3, 1, 3← 2, 1, 2	Ground						28 607.4	.2	165
		3, 2, 1← 2, 2, 0	Ground						28 661.7	.2	165
		3, 2, 1← 2, 2, 0	Ground						28 705.6	.2	165
		3, 2, 2← 2, 2, 1	Ground						28 645.7	.2	165
$C^{12}D_3C^{12}F_3^{19}$	414	2, ← 1,	Ground						18 423.6	.2	165
		2, ← 1,	Ground						27 510.5	.2	165
		2, ← 1,	Ground						27 563.0	.2	165
		2, ← 1,	Ground						27 597.5	.2	165
		3, ← 2,	Ground						27 635.9	.2	165

C_2H_3NS $C_s(C_{3v},C_s)$ CH_3NCS

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3N^{14}C^{12}S^{32}$	C_s	421	78 200. M	2 548. M	2 506. M	.0036	.4020		

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
421	3.18 T		0. X					300 1	600 1		

References:

ABC: 20 D_J: 20 D_{JK}: 20 κ: Δ:

μ: 395 eQq: V: I: ω: 20

Torsional frequency = 200 cm^{-1}. Ref: 20.

Methyl Isothiocyanate Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a ; v_b	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3N^{14}C^{12}S^{32}$	421	4, , ← 3, ,	Ground						20 216.		20
		4, , ← 3, ,	0; 1						20 241.		20
		4, , ← 3, ,	1; 0						20 350.		20
		4, , ← 3, ,		1					20 443.		20
		4, 1, 4← 3, 1, 3	Ground						20 140.		20
		5, , ← 4, ,	Ground						25 269.		20
		5, , ← 4, ,	0; 1						25 306.		20
		5, , ← 4, ,	1; 0						25 442.		20
		5, , ← 4, ,		1					25 550.		20
		5, 1, 4← 4, 1, 3	Ground						25 333.		20
		5, 1, 4← 4, 1, 3		1					25 653.		20
		5, 1, 5← 4, 1, 4	Ground						25 195.		20
$C^{13}H_3N^{14}C^{12}S^{32}$	422	5, , ← 4, ,	Ground						24 143.		20
$C^{12}H_3N^{14}C^{13}S^{32}$	423	5, , ← 4, ,	Ground						25 002.		20
$C^{12}H_3N^{14}C^{12}S^{33}$	424	5, , ← 4, ,	Ground						24 930.		20
$C^{12}H_3N^{14}C^{12}S^{34}$	425	4, , ← 3, ,	Ground						19 700.		20
		4, , ← 3, ,		1					19 929.		20
		5, , ← 4, ,	Ground						24 609.		20
		5, , ← 4, ,		1					24 910.		20
		6, , ← 5, ,	Ground						29 540.		20
		6, , ← 5, ,	Ground						29 700.		20
$C^bH_3^bN^bC^bS^b$	426	4, , ← 3, ,							20 020.		20
		4, , ← 3, ,							20 230.		20
		4, , ← 3, ,							20 413.		20
		5, , ← 4, ,							24 824.		20
		5, , ← 4, ,							24 971.		20
		5, , ← 4, ,							25 077.		20
		5, , ← 4, ,							25 100.		20
		5, , ← 4, ,							25 161.		20
		5, , ← 4, ,							25 390.		20
		5, , ← 4, ,							25 409.		20

C_2H_3NS $C_s(C_{3v},C_s)$ CH_3SCN

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3S^{32}C^{12}N^{14}$	C_s	431							

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
431	3.16 T		0. X								

References:

ABC: D_J: D_{JK}: κ: Δ:

μ: 395 eQq: V: I: ω:

The average rotational constant (B + C)/2 is: .09462 ± .00005 cm^{-1}. Ref: 20.

Methyl Thiocyanate

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3S^{32}C^{12}N^{14}$	431	4, , ← 3, ,	Excited						22 680.	10.	20
		5, , ← 4, ,	Excited						28 380.	10.	20

C_2H_4ClF $C_1(C_s,C_s)$ CH_2FCH_2Cl

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$F^{19}H_2C_2^{12}H_2Cl^{35}$	C_1	441	13 606.45 M	3 289.9 M	2 876.75 M			−.923	
$F^{19}H_2C_2^{12}H_2Cl^{37}$	C_1	442						−.9262	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
441		1.97[1] T									

1. Dipole moments given in Maryott and Buckley range from 1.84 to 1.97 D. Since the cis- form would be expected to yield a higher value for the dipole moment, that value is quoted here.

References:

ABC: 231 D_J: D_{JK}: κ: 231, 259 Δ:

μ: 393 eQq: V: I: ω:

Add. Ref.: 185

For species 441, $\chi_{aa}=-23.5$ MHz, $\chi_{bb}=-8.8$ MHz, and $\chi_{cc}=32.3$ MHz. Ref: 231.
For species 442, $\chi_{aa}=-17.6$ MHz, $\chi_{bb}=-6.1$ MHz, and $\chi_{cc}=23.7$ MHz, and $A-C=10744.55$ MHz. Ref: 259.

1-Chloro-2-Fluoroethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$F^{19}H_2C_2^{12}H_2Cl^{35}$	441	1, 1, 0← 1, 0, 1	Ground						10 729.7	.1	231
		2, 1, 2← 1, 0, 1	Ground						22 236.7	.1	231
		2, 1, 1← 2, 0, 2	Ground						11 155.	.1	231
		3, 1, 3← 2, 0, 2	Ground						27 786.4	.1	231
		3, 1, 2← 3, 0, 3	Ground						11 815.4	.1	231
		4, 0, 4← 3, 1, 3	Ground						15 204.6	.1	231
		4, 1, 3← 4, 0, 4	Ground						12 736.4	.1	231
		5, 0, 5← 4, 1, 4	Ground						21 979.4	.1	231
		5, 1, 4← 5, 0, 5	Ground						13 952.1	.1	231
		6, 0, 6← 5, 1, 5	Ground						28 812.	.1	231
		6, 1, 5← 6, 0, 6	Ground						15 500.3	.1	231
$F^{19}H_2C_2^{12}H_2Cl^{37}$	442	1, 1, 0← 1, 0, 1	Ground						10 744.55		259
		2, 1, 1← 2, 0, 2	Ground						11 152.15		259
		3, 1, 2← 3, 0, 3	Ground						11 784.5		259
		4, 1, 3← 4, 0, 4	Ground						12 665.0		259
		5, 1, 4← 5, 0, 5	Ground						13 825.4		259

1. An apparent misprint in one of the transitions given in Mukhtarov's article has been assumed to mean $3_{13}\leftarrow 2_{02}$ rather than $3_{13}\leftarrow 2_{03}$.

$C_2H_4Cl_2$ $C_s(C_s,C_s)$ CH_2ClCH_2Cl

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
g-$C^{12}H_2Cl^{35}C^{12}H_2Cl^{35}$	C_2	451	9 299. [2]M	2 510. [2]M	2 090. [2]M			−.883	
g-$C^{12}H_2Cl^{35}C^{12}H_2Cl^{37}$	C_2	452	9 239. [2]M	2 447. [2]M	2 032. [2]M			−.884	
g-$C^{12}H_2Cl^{37}C^{12}H_2Cl^{37}$	C_2	453	9 180. [2]M	2 385. [2]M	1 974. [2]M			−.885	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
451	0. X	1.60[1] T	0. X								

1. The dipole moment of the gauche form must occur along the axis of symmetry of the molecule, which in this case is the b-axis. Widely varying dipole moment values are given in references, indicating that it is poorly known. One of the higher values was chosen since the gauche form would be expected to have a higher dipole moment.
2. The rotational constants were based upon "possible" identification of observed lines.

References:

ABC: 134 D_J: D_{JK}: κ: 134 Δ:

μ: 393 eQq: V: I: ω:

1,2-Dichloroethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
g-$C^{12}H_2Cl^{35}C^{12}H_2Cl^{35}$	451	2, 2, 1← 1, 1, 0							30 190.		134 [1]
		3, 2, 2← 2, 1, 1							34 418.		134 [1]
		5, 1, 5← 4, 0, 4							27 289.		134 [1]
		6, 1, 6← 5, 0, 5							30 992.		134 [1]
		11, 1,10←11, 0,11							27 160.		134 [1]
		12, 1,11←12, 0,12							30 650.		134 [1]

1. The authors state that these identifications of the observed lines are "possible".

$C_2H_4F_2$ $C_s(C_{3v},C_s)$ CH_3CHF_2

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}HF_2^{19}$	C_s	461	9 491.95 M	8 962.65 M	5 170.43 M			.75504	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
461	2.01 M	0. X	1.12 M		3180		5.122	395 1			

References:

ABC: 98 D_J: D_{JK}: κ: 98 Δ:

μ: 292 eQq: V: 258 I: 98 ω: 98

Torsional frequency = 235 cm^{-1}. Ref: 98.

1,1-Difluoroethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}HF_2^{19}$	461	1, 1, 0← 0, 0, 0	Ground	1					18 425.9		137
		1, 1, 0← 0, 0, 0	Ground						18 454.7	.1	98
		2, 0, 2← 1, 0, 1	1						24 894.3	.1	98
		2, 0, 2← 1, 0, 1	Ground	1					24 926.6		137
		2, 0, 2← 1, 0, 1	Ground						24 951.6	.1	98
		2, 1, 1← 1, 0, 1	Ground	1					31 966.3		137
		2, 1, 1← 1, 0, 1	Ground						36 379.9	.1	98
		2, 1, 1← 1, 1, 0	Ground						32 049.0	.1	98
		2, 1, 2← 1, 1, 1	1						24 382.5	.1	98
		2, 1, 2← 1, 1, 1	Ground	1					24 425.7		137
		2, 1, 2← 1, 1, 1	Ground						24 473.8	.1	98
		2, 2, 0← 1, 1, 0	Ground						36 959.4	.1	98
		2, 2, 1← 1, 1, 1	Ground						37 438.4	.1	98
		3, 0, 2← 2, 0, 1	Ground						35 097.0	.1	98
		3, 1, 3← 2, 1, 2	Ground						35 049.0	.1	98
		3, 1, 2← 3, 1, 3	Ground						20 059.7	.1	98
		3, 2, 2← 3, 0, 3	Ground						20 317.9	.1	98
		4, 1, 3← 4, 1, 4	Ground						28 290.1	.1	98
		4, 2, 3← 4, 0, 4	Ground						28 312.4	.1	98
		4, 2, 2← 4, 2, 3	Ground						19 705.1	.1	98
		4, 3, 2← 4, 1, 3	Ground						20 470.9	.1	98
		5, 1, 4← 5, 1, 5	Ground						36 403.3	.1	98
		5, 2, 4← 5, 0, 5	Ground						36 403.3	.1	98
		5, 2, 3← 5, 2, 4	Ground						28 192.1	.1	98
		5, 3, 3← 5, 1, 4	Ground						28 280.6	.1	98

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}HF_2^{19}$	461	5, 3, 2← 5, 3, 3	Ground							19 055.8	.1	98
		5, 4, 2← 5, 2, 3	Ground							20 796.2	.1	98
		6, 2, 4← 6, 2, 5	Ground							36 351.2	.1	98
		6, 3, 4← 6, 1, 5	Ground							36 358.5	.1	98
		6, 3, 3← 6, 3, 4	Ground							27 991.3	.1	98
		6, 4, 3← 6, 2, 4	Ground							28 254.8	.1	98
		6, 4, 2← 6, 4, 3	Ground							18 061.2	.1	98
		6, 5, 2← 6, 3, 3	Ground							21 399.2	.1	98
		6, 5, 2← 6, 3, 3	Ground	A	1					21 496.7		137
		6, 5, 2← 6, 3, 3	Ground	E	1					21 498.2		137
		7, 3, 4← 7, 3, 5	Ground							36 263.9	.1	98
		7, 4, 4← 7, 2, 5	Ground							36 291.4	.1	98
		7, 4, 3← 7, 4, 4	Ground							27 618.3	.1	98
		7, 5, 3← 7, 3, 4	Ground							28 265.6	.1	98
		7, 6, 2← 7, 4, 3	Ground							22 423.1		137
		7, 6, 2← 7, 4, 3	Ground	A	1					22 635.8		137
		7, 6, 2← 7, 4, 3	Ground	E	1					22 638.0		137
		8, 5, 3← 8, 5, 4	Ground	E	1					26 740.4		137
		8, 5, 3← 8, 5, 4	Ground	A	1					26 741.1		137
		8, 5, 3← 8, 5, 4	Ground							26 985.8	.1	98
		8, 6, 3← 8, 4, 4	Ground							28 364.6	.1	98
		8, 7, 2← 8, 5, 3	Ground							23 996.4		137
		8, 7, 2← 8, 5, 3	Ground	A	1					24 408.7		137
		8, 7, 2← 8, 5, 3	Ground	E	1					24 412.3		137
		9, 7, 3← 9, 5, 4	Ground							28 630.2	.1	66
		9, 8, 2← 9, 6, 3	Ground							26 303.3		137
		9, 8, 2← 9, 6, 3	Ground	A	1					26 977.9		137
		9, 8, 2← 9, 6, 3	Ground	E	1					26 983.1		137
		10, 7, 3←10, 7, 4	Ground	E	1					24 099.1		137
		10, 7, 3←10, 7, 4	Ground	A	1					24 101.7		137
		10, 7, 3←10, 7, 4	Ground							24 621.7		137
		11, 8, 3←11, 8, 4	Ground	E	1					22 136.3		137
		11, 8, 3←11, 8, 4	Ground	A	1					22 139.7		137
		11, 8, 3←11, 8, 4	Ground							22 822.2		137
		12, 9, 3←12, 9, 4	Ground	E	1					19 813.4		137
		12, 9, 3←12, 9, 4	Ground	A	1					19 818.0		137
		12, 9, 3←12, 9, 4	Ground							20 662.0		137

C_2H_4O $C_s(C_{3v},C_s)$ CH_3CHO

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}HO^{16}$	C_s	471	56 920.5 M	10 165.1 M	9 100.0 M	−.0028			
$C^{12}D_3C^{12}DO^{16}$	C_s	472	34 990.6 M	8 577.9 M	7 531.4 M	−.0021			
s-$C^{12}H_2DC^{12}HO^{16}$	C_s	473		9 864.80 M	8 637.07 M				
$C^{12}D_3C^{12}HO^{16}$	C_s	474	41 798. M	8 590.23 M	7 816.87 M	−.0023			
s-$C^{12}HD_2C^{12}HO^{16}$	C_s	475		8 779.55 M	8 174.35 M				
$C^{13}H_3C^{12}HO$	C_s	476	56 757.22 M	9 857.50 M	8 848.74 M				
$C^{12}H_3C^{13}HO^{16}$	C_s	477	55 816.3 M	10 162.6 M	9 069.6 M				
$C^{13}H_3C^{13}HO^{16}$	C_s	478	55 650.1 M	9 853.46 M	8 818.68 M				
$C^{12}H_3C^{12}HO^{18}$	C_s	479	56 267. M	9 677.77 M	8 692.46 M	−.0028			

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
471	2.55 M	0.87 M	0. X		1162	30					
472					1151	30					
474					1143	39					

References:

ABC: 171 D_J: 171 D_{JK}: κ: Δ:

μ: 171 eQq: V: 171 I: ω:

Add. Refs.: 23, 51, 144, 236

For species 471, $V_6 < 50$ cal/mol. For species 472, $V_6 < 58$ cal/mol. For species 474, $V_6 < 39$ cal/mol. Ref: 171.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}HO^{16}$	471	1, 0, 1← 0, 0, 0	Ground	A	0					19 225.7	.2	171
		1, 0, 1← 0, 0, 0	Ground	E	0					19 262.3	.3	171
		1, 0, 1← 0, 0, 0	Ground	A	0					19 265.3	.2	171
		1, 0, 1← 0, 0, 0	Ground	A	0					19 268.27	.2	171
		2, 0, 2← 1, 0, 1	Ground	E	0					38 506.4	.4	171
		2, 0, 2← 1, 0, 1	Ground	A	0					38 512.3	.3	171
		2, 0, 2← 1, 0, 1	Ground	A	0					38 522.86	.3	171
		2, 0, 2← 1, 1, 1	Ground	A	0					8 243.0	.5	171
		2, 1, 1← 1, 1, 0	Ground	E	0					39 362.46	.4	171
		2, 1, 1← 1, 1, 0	Ground	A	0					39 454.94	.3	171
		2, 1, 1← 1, 1, 0	Ground	A	0					39 594.86	.3	171
		2, 1, 2← 1, 1, 1	Ground	A	0					37 464.58	.3	171
		2, 1, 2← 1, 1, 1	Ground	A	0					37 515.24	.3	171
		2, 1, 2← 1, 1, 1	Ground	E	0					37 687.18	.4	171
		3, 0, 3← 2, 1, 2	Ground	A	0					12 015.05	.2	171
		3, 0, 3← 2, 1, 2	Ground	E	0					12 666.62	.4	171
		4, 0, 4← 3, 1, 3	Ground	A	0					32 709.25	.2	171
		5, 1, 4← 5, 1, 5	Ground	A	0					15 968.60	.2	171
		5, 1, 4← 5, 1, 5	Ground	E	0					15 988.80	.3	171
		6, 1, 5← 6, 1, 6	Ground	E	0					22 326.56	.3	171
		6, 1, 5← 6, 1, 6	Ground	A	0					22 346.18	.2	171
		7, 1, 6← 7, 1, 7	Ground	E	0					29 718.83	.3	171
		7, 1, 6← 7, 1, 7	Ground	A	0					29 774.15	.2	171
		8, 1, 7← 8, 1, 8	Ground	E	0					38 151.3	.4	171
		8, 1, 7← 8, 1, 8	Ground	A	0					38 241.2	.3	171
		11, 2, 9←11, 2,10	Ground	A	0					12 158.31	.2	171
		12, 2,10←12, 2,11	Ground	A	0					16 682.08	.2	171
		13, 2,11←13, 2,12	Ground	A	0					22 208.47	.2	171
		14, 2,12←14, 2,13	Ground	A	0					28 797.83	.2	171
		Not Reported	Ground							8 723.11		141
		Not Reported	Ground							12 338.17		141
		Not Reported	Ground							12 366.25		141
		Not Reported								12 381.40		141
		Not Reported								12 391.52		141
		Not Reported								16 541.75		141
		Not Reported								16 551.01		141
		Not Reported	Ground							16 657.45		141
		Not Reported	Ground							16 870.93		141
		Not Reported	Ground							16 913.79		141
		Not Reported								17 018.35		141
		Not Reported								20 650.80		141
		Not Reported								20 701.5		141
		Not Reported								21 640.36		141
		Not Reported								21 651.27		141
		Not Reported								21 768.25		141
		Not Reported								22 087.00		141
		Not Reported								22 234.82		141
		Not Reported								22 313.79		141
		Not Reported								22 464.77		141
		Not Reported								22 738.93		141

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}HO^{16}$	471	Not Reported								22 986.53		141
		Not Reported								23 364.79		141
		Not Reported								23 553.26		141
		Not Reported								23 577.38		141
		Not Reported								27 206.96		141
		Not Reported								27 214.44		141
		Not Reported								27 231.02		141
		Not Reported								27 445.4		141
		Not Reported								27 526.04		141
		Not Reported								27 773.33		141
		Not Reported								28 330.59		141
		Not Reported								28 788.00		141
		Not Reported								28 789.01		141
		Not Reported								28 920.40		141
		Not Reported								28 974.95		141
		Not Reported								29 077.76		141
		Not Reported								29 093.30		141
		Not Reported								29 123.5		141
		Not Reported								29 396.99		141
		Not Reported								29 832.		141
		Not Reported								30 830.61		141
		Not Reported								33 312.64		141
		Not Reported								34 711.88		141
		Not Reported								35 320.94		141
		Not Reported								36 489.52		141
		Not Reported								36 602.12		141
		Not Reported								36 613.28		141
		Not Reported								37 291.0		141
		Not Reported	Ground	A	0					37 708.80	.3	171
		Not Reported								38 339.24		141
		Not Reported								38 833.0		141
$C^{12}D_3C^{12}DO^{16}$	472	1, 0, 1← 0, 0, 0	Ground	A	0					16 109.59	.1	171
		1, 0, 1← 0, 0, 0	Ground	A	0					16 116.45	.5	171
		1, 0, 1← 1, 1, 0	Ground	E	0					27 430.55	.4	171
		1, 0, 1← 1, 1, 0	Ground	A	0					27 459.13	.2	171
		2, 0, 2← 1, 0, 1	Ground	E	0					32 187.05	.1	171
		2, 0, 2← 1, 0, 1	Ground	A	0					32 187.52	.1	171
		2, 1, 1← 1, 1, 0	Ground	E	0					33 262.94	.1	171
		2, 1, 1← 1, 1, 0	Ground	A	0					33 264.34	.1	171
		2, 1, 2← 1, 1, 1	Ground	A	0					31 171.36	.2	171
		2, 0, 2← 2, 1, 1	Ground	E	0					28 506.78	.4	171
		2, 0, 2← 2, 1, 1	Ground	A	0					28 536.30	.2	171
		3, 0, 3← 2, 1, 2	Ground	A	0					22 808.47	.2	171
		3, 0, 3← 2, 1, 2	Ground	E	0					22 837.22	.4	171
		6, 1, 5← 6, 1, 6	Ground	E	0					21 919.74	.3	171
		6, 1, 5← 6, 1, 6	Ground	A	0					21 926.40	.2	171
		7, 1, 6← 7, 1, 7	Ground	E	0					29 170.90	.4	171
		7, 1, 6← 7, 1, 7	Ground	A	0					29 179.77	.2	171
		8, 1, 7← 8, 1, 8	Ground	E	0					37 397.40	.4	171

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3C^{12}DO^{16}$	472	8, 1, 7← 8, 1, 8	Ground	A	0					37 409.18	.3	171
		11, 2, 9←11, 2,10	Ground	A	0					18 844.55	.2	171
		11, 2, 9←11, 2,10	Ground	E	0					18 849.74	.3	171
		12, 2,10←12, 2,11	Ground	A	0					25 228.77	.1	171
		12, 2,10←12, 2,11	Ground	E	0					25 234.17	.2	171
		13, 2,11←13, 2,12	Ground	A	0					32 720.26	.1	171
		13, 2,11←13, 2,12	Ground	E	0					32 726.13	.5	171
		Not Reported								18 963.78		141
		Not Reported								21 819.28		141
		Not Reported								22 756.43		141
		Not Reported								26 433.48		141
		Not Reported								26 445.68		141
		Not Reported								26 481.08		141
		Not Reported								26 494.55		141
		Not Reported								26 666.14		141
		Not Reported								26 772.7		141
		Not Reported								29 186.9		141
		Not Reported								29 221.05		141
s-$C^{12}H_2DC^{12}HO^{16}$	473	1, 0, 1← 0, 0, 0	Ground							18 501.87	.1	171
		1, 0, 1← 0, 0, 0	Ground							18 504.36	.1	171
		1, 0, 1← 0, 0, 0	Ground							18 677.30	.2	171
		1, 0, 1← 0, 0, 0	Ground							18 679.28	.2	171
		2, 0, 2← 1, 0, 1	Ground							36 975.	3.	171
		2, 0, 2← 1, 0, 1	Ground							36 981.7	.3	171
		2, 1, 1← 1, 1, 0	Ground							38 187.2	.5	171
		2, 1, 1← 1, 1, 0	Ground							38 231.25	.5	171
		2, 1, 2← 1, 1, 1	Ground							35 775.8	.3	171
		4, 1, 3← 4, 1, 4	Ground							12 273.5	.3	171
		4, 1, 3← 4, 1, 4	Ground							12 660.45	.2	171
		5, 1, 4← 5, 1, 5	Ground							18 402.40	.3	171
		5, 1, 4← 5, 1, 5	Ground							18 594.39	.2	171
		6, 1, 5← 6, 1, 6	Ground							25 748.55	.3	171
		6, 1, 5← 6, 1, 6	Ground							25 889.3	.5	171
		6, 1, 5← 6, 1, 6	Ground							25 917.11	.2	171
		Not Reported								12 706.25		141
		Not Reported								16 938.2		141
		Not Reported								17 234.91		141
		Not Reported								17 263.05		141
		Not Reported								17 777.2		141
		Not Reported								17 868.8		141
		Not Reported								18 991.57		141
		Not Reported								22 978.		141
		Not Reported								25 724.83		141
		Not Reported								26 105.14		141
		Not Reported								28 571.69		141
		Not Reported								28 586.2		141
		Not Reported								29 467.7		141
		Not Reported								29 550.43		141

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3C^{12}HO^{16}$	474	1, 0, 1← 0, 0, 0	Ground	A	0					16 407.00	.2	171
		2, 0, 2← 1, 0, 1	Ground	E	0					32 799.89	.4	171
		2, 0, 2← 1, 0, 1	Ground	A	0					32 801.27	.2	171
		2, 0, 2← 1, 0, 1	Ground	A	0					32 854.7		171
		2, 1, 1← 1, 0, 1	Ground	A	0					33 587.42	.2	171
		2, 1, 1← 1, 1, 0	Ground	E	0					33 577.06	.4	171
		2, 1, 2← 1, 1, 1	Ground	A	0					32 040.91	.1	171
		2, 1, 2← 1, 1, 1	Ground	E	0					32 050.00	2.	171
		4, 1, 3← 4, 0, 4	Ground	E	0					37 527.60	.5	171
		4, 1, 3← 4, 0, 4	Ground	A	0					37 626.28	.3	171
		5, 1, 4← 5, 0, 5	Ground	E	0					39 664.22	.5	171
		5, 1, 4← 5, 0, 5	Ground	A	0					39 763.40	.3	171
		6, 1, 5← 6, 1, 6	Ground	E	0					16 208.84	.5	171
		6, 1, 5← 6, 1, 6	Ground	A	0					16 224.33	.3	171
		7, 1, 6← 7, 1, 7	Ground	E	0					21 596.15	.4	171
		7, 1, 6← 7, 1, 7	Ground	A	0					21 616.82	.2	171
		8, 1, 7← 8, 1, 8	Ground	E	0					27 736.32	.4	171
		8, 1, 7← 8, 1, 8	Ground	A	0					27 762.42	.2	171
		13, 2,11←13, 2,12	Ground	A	0					16 433.52	.3	171
		13, 2,11←13, 2,12	Ground	E	0					16 442.90	.5	171
		14, 2,12←14, 2,13	Ground	A	0					21 292.13	.3	171
		14, 2,12←14, 2,13	Ground	E	0					21 303.65	.4	171
s-$C^{12}HD_2C^{12}HO^{16}$	475	1, 0, 1← 0, 0, 0	Ground							16 953.90	.2	171
		1, 0, 1← 0, 0, 0	Ground							16 990.04	.2	171
		1, 0, 1← 0, 0, 0	Ground							17 056.65	.3	171
		2, 1, 2← 1, 1, 1	Ground							33 302.30	.3	171
		7, 1, 6← 7, 1, 7	Ground							16 926.85	.2	171
		8, 1, 7← 8, 1, 8	Ground							21 752.05	.2	171
		9, 1, 8← 9, 1, 9	Ground							21 170.68	.2	171
$C^{13}H_3C^{12}HO$	476	1, 0, 1← 0, 0, 0	Ground	E	0					18 703.69	.1	171
		1, 0, 1← 0, 0, 0	Ground	A	0					18 706.46	.1	171
		2, 0, 2← 1, 0, 1	Ground	E	0					37 391.12	.2	171
		2, 0, 2← 1, 0, 1	Ground	A	0					37 396.36	.2	171
		2, 0, 2← 1, 1, 1	Ground	A	0					9 513.06	.2	171
		2, 1, 1← 1, 1, 0	Ground	E	0					38 186.94	.3	171
		2, 1, 1← 1, 1, 0	Ground	A	0					38 420.36	.1	171
		2, 1, 2← 1, 1, 1	Ground	A	0					36 402.86	.3	171
		2, 1, 2← 1, 1, 1	Ground	E	0					36 628.12	.5	171
		3, 0, 3← 2, 1, 2	Ground	A	0					10 146.83	.2	171
		4, 0, 4← 3, 1, 3	Ground	A	0					30 216.05	.2	171
$C^{12}H_3C^{13}HO^{16}$	477	1, 0, 1← 0, 0, 0	Ground	E	0					19 229.94	.2	171
		1, 0, 1← 0, 0, 0	Ground	A	0					19 232.43	.3	171
		2, 0, 2← 1, 0, 1	Ground	E	0					38 439.56	.2	171
		2, 0, 2← 1, 0, 1	Ground	A	0					38 445.38	.2	171
		2, 1, 1← 1, 1, 0	Ground	E	0					39 343.4	.5	171
		2, 1, 1← 1, 1, 0	Ground	A	0					39 557.00	.3	171
		2, 1, 2← 1, 1, 1	Ground	A	0					37 370.9	.2	171
		2, 1, 2← 1, 1, 1	Ground	E	0					37 574.6	1.	171

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{13}HO^{16}$	477	3, 0, 3← 2, 1, 2	Ground	A	0					13 039.14	.2	171
		4, 0, 4← 3, 1, 3	Ground	A	0					33 725.	1.	171
$C^{13}H_3C^{13}HO^{16}$	478	1, 0, 1← 0, 0, 0	Ground	E	0					18 670.03	.3	171
		1, 0, 1← 0, 0, 0	Ground	A	0					18 672.20	.2	171
		2, 0, 2← 1, 0, 1	Ground	E	0					37 322.20	.2	171
		2, 0, 2← 1, 0, 1	Ground	A	0					37 326.98	.2	171
		2, 1, 1← 1, 1, 0	Ground	E	0					38 164.5	.4	171
		2, 1, 1← 1, 1, 0	Ground	A	0					38 378.82	.2	171
		2, 1, 2← 1, 1, 1	Ground	A	0					36 309.26	.3	171
		2, 1, 2← 1, 1, 1	Ground	E	0					36 515.58	.2	171
		3, 0, 3← 2, 1, 2	Ground	A	0					11 167.75	.2	171
		4, 0, 4← 3, 1, 3	Ground	A	0					31 229.94	.2	171
$C^{12}H_3C^{12}HO^{18}$	479	1, 0, 1← 0, 0, 0	Ground	E	0					18 367.75	.5	171
		1, 0, 1← 0, 0, 0	Ground	A	0					18 370.23	.5	171
		2, 0, 2← 1, 0, 1	Ground	E	0					36 719.90	.4	171
		2, 0, 2← 1, 0, 1	Ground	A	0					36 725.26	.4	171
		2, 1, 1← 1, 1, 0	Ground	A	0					37 724.4	1.	171
		5, 1, 4← 5, 1, 5	Ground	A	0					14 772.90	.3	171
		6, 1, 5← 6, 1, 6	Ground	A	0					20 674.05	.2	171
		7, 1, 6← 7, 1, 7	Ground	A	0					27 547.7	.5	171
a-$C^{12}H_2DC^{12}HO^{16}$	481	1, 0, 1← 0, 0, 0	Ground							18 001.96	.2	171
		1, 0, 1← 0, 0, 0	Ground							18 005.15	.2	171
		1, 0, 1← 0, 0, 0	Ground							18 043.35	.3	171
		1, 0, 1← 0, 0, 0	Ground							18 263.51	.3	171
		1, 0, 1← 0, 0, 0	Ground							18 350.10	.3	171
		2, 0, 2← 1, 0, 1	Ground							35 989.85	.3	171
		2, 0, 2← 1, 0, 1	Ground							35 991.70	.3	171
		2, 1, 1← 1, 1, 0	Ground							36 799.	3.	171
		2, 1, 2← 1, 1, 1	Ground							35 206.37	.5	171
		2, 1, 2← 1, 1, 1	Ground							35 321.1	.5	171
		5, 1, 4← 5, 1, 5	Ground							12 319.72	.3	171
		5, 1, 4← 5, 1, 5	Ground							12 339.69	.2	171
		6, 1, 5← 6, 1, 6	Ground							17 234.91	.3	171
		6, 1, 5← 6, 1, 6	Ground							17 263.05	.2	171
		7, 1, 6← 7, 1, 7	Ground							22 964.06	.2	171
		7, 1, 6← 7, 1, 7	Ground							23 000.94	.2	171
		8, 1, 7← 8, 1, 8	Ground							29 500.67	.2	171
		8, 1, 7← 8, 1, 8	Ground							29 548.31	.2	171
a-$C^{12}HD_2C^{12}HO^{16}$	482	1, 0, 1← 0, 0, 0	Ground							17 363.35	.2	171
		1, 0, 1← 0, 0, 0	Ground							17 387.12	.3	171
		2, 0, 2← 1, 0, 1	Ground							34 706.02	.2	171
		2, 0, 2← 1, 0, 1	Ground							34 707.32	.2	171
		2, 1, 1← 1, 1, 0	Ground							35 711.86	.3	171
		2, 1, 2← 1, 1, 1	Ground							33 741.3	.5	171
		5, 1, 4← 5, 1, 5	Ground							14 827.5	.3	171
		5, 1, 4← 5, 1, 5	Ground							14 839.05	.3	171
		6, 1, 5← 6, 1, 6	Ground							20 746.48	.2	171
		6, 1, 5← 6, 1, 6	Ground							20 761.20	.2	171
		7, 1, 6← 7, 1, 7	Ground							27 634.90	.5	171
		7, 1, 6← 7, 1, 7	Ground							27 655.01	.2	171

$C_2H_4O_2$ $C_s(C_{3v},C_s,C_s)$ CH_3COOH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}O^{16}O^{16}H$	C_s	491	11 073. M	9 056. M	4 864. M				
$C^{12}D_3C^{12}O^{16}O^{16}H$	C_s	492							

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
491		1.74 T	0. X		496						
492					467						

References:

ABC: 145 D_J: D_{JK}: κ: Δ:

μ: 393 eQq: V: 193 I: ω:

Add. Ref.: 75

Rotational constants for the excited state: A = 11139 MHz, B = 9110 MHz, and C = 4868 MHz. Ref: 145.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}O^{16}H$	491	1, 1, 1← 0, 0, 0	Ground	E	0					16 418.82	.4	193
		1, 1, 1← 0, 0, 0	Ground	A	0					16 741.72	.4	193
		2, 0, 2← 1, 0, 1	Ground							25 091.	3.	145
		2, 0, 2← 1, 0, 1	Excited							25 171.	3.	145
		2, 0, 2← 1, 1, 1	Excited							23 138.	3.	145
		2, 0, 2← 1, 1, 1	Ground	A	0					24 920.64	.4	193
		2, 0, 2← 1, 1, 1	Ground	E	0					25 156.42	.4	193
		2, 1, 2← 1, 0, 1	Excited							25 742.	3.	145
		2, 1, 2← 1, 0, 1	Ground	E	0					27 205.64	.4	193
		2, 1, 2← 1, 0, 1	Ground	A	0					27 394.12	.4	193
		2, 1, 2← 1, 1, 1	Ground							23 648.	3.	145
		2, 1, 2← 1, 1, 1	Excited							23 713.	3.	145
		2, 1, 1← 2, 0, 2	Ground							12 989.83		382
		2, 2, 1← 2, 1, 2	Ground							18 625.	3.	145
		2, 2, 1← 2, 1, 2	Excited							18 814.	3.	145
		3, 1, 2← 3, 0, 3	Ground							23 540.87		382
		3, 2, 1← 3, 1, 2	Ground	A	0					12 398.58	.4	193
		3, 3, 0← 3, 2, 1	Ground							12 984.48		382
		4, 2, 2← 4, 1, 3	Ground							21 463.58		382
		4, 3, 1← 4, 2, 2	Ground							13 381.79		382
		5, 2, 3← 5, 1, 4	Ground							33 021.39		382
		5, 4, 1← 5, 3, 2	Ground	A	0					16 539.43	.4	193
		5, 4, 2← 5, 3, 3	Ground							29 391.68		382
		6, 3, 3← 6, 2, 4	Ground							30 521.46		382
		6, 4, 2← 6, 3, 3	Ground							18 807.79		382
		6, 5, 1← 6, 4, 2	Ground	A	0					22 082.56	.4	193
		7, 4, 3← 7, 3, 4	Ground							27 525.60		382
		7, 5, 2← 7, 4, 3	Ground							20 357.84		382
		7, 6, 1← 7, 5, 2	Ground	A	0					29 522.57	.4	193
		8, 5, 3← 8, 4, 4	Ground							25 240.46		382
		8, 5, 3← 8, 5, 4	Ground							20 209.32		382
		8, 6, 2← 8, 5, 3	Ground							24 587.82		382
		9, 6, 3← 9, 5, 4	Ground	A	0					24 949.51	.4	193
		9, 6, 3← 9, 6, 4	Ground							14 577.35		382
		10, 7, 3←10, 6, 4	Ground							27 444.98		382
		Not Reported								22 324.	3.	145
		Not Reported								22 356.	3.	145
		Not Reported								22 542.	3.	145
		Not Reported								22 583.	3.	145
		Not Reported								22 616.	3.	145
		Not Reported								22 681.	3.	145
		Not Reported								22 827.	3.	145
		Not Reported								22 943.	3.	145
		Not Reported								22 968.	3.	145
		Not Reported								23 042.	3.	145
		Not Reported								23 179.	3.	145
		Not Reported								23 317.	3.	145
		Not Reported								23 405.	3.	145
		Not Reported								23 422.	3.	145
		Not Reported								23 426.	3.	145

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}O^{16}H$	491	Not Reported								23 429.	3.	145
		Not Reported								23 471.	3.	145
		Not Reported								23 574.	3.	145
		Not Reported								23 623.	3.	145
		Not Reported								23 703.	3.	145
		Not Reported								23 717.	3.	145
		Not Reported								23 809.	3.	145
		Not Reported								23 813.	3.	145
		Not Reported								23 819.	3.	145
		Not Reported								23 966.	3.	145
		Not Reported								24 132.	3.	145
		Not Reported								24 208.	3.	145
		Not Reported								24 298.	3.	145
		Not Reported								24 334.	3.	145
		Not Reported								24 340.	3.	145
		Not Reported								24 385.	3.	145
		Not Reported								24 456.	3.	145
		Not Reported								24 968.	3.	145
		Not Reported								25 083.	3.	145
		Not Reported								25 320.	3.	145
		Not Reported								25 327.	3.	145
		Not Reported								25 339.	3.	145
		Not Reported								25 506.	3.	145
$C^{12}D_3C^{12}O^{16}O^{16}H$	492	1, 1, 1← 0, 0, 0		E	0					15 329.70	.4	193
		1, 1, 1← 0, 0, 0		A	0					15 364.93	.4	193
		2, 0, 2← 1, 1, 1		A	0					20 964.23	.4	193
		2, 0, 2← 1, 1, 1		E	0					20 992.55	.4	193
		2, 1, 2← 1, 0, 1		E	0					24 871.11	.4	193
		2, 1, 2← 1, 0, 1		A	0					24 902.31	.4	193
		2, 1, 2← 3, 0, 3	Ground							32 068.90		382
		2, 1, 2← 3, 0, 3	Ground							32 076.50		382
		3, 1, 3← 2, 0, 2		E	0					33 596.36	.4	193
		3, 1, 3← 2, 0, 2		A	0					33 621.42	.4	193
		6, 4, 2← 6, 3, 3	Ground							19 495.85		382
		7, 3, 4← 7, 2, 5	Ground							30 800.79		382
		7, 4, 3← 7, 3, 4	Ground							20 773.23		382
		7, 5, 2← 7, 4, 3	Ground							26 773.22		382
		8, 4, 4← 8, 3, 5	Ground							26 870.71		382
		9, 5, 4← 9, 4, 5	Ground							25 422.18		382
		11, 6, 5←11, 5, 6	Ground							30 008.04		382

$C_2H_4O_2$ $C_s(C_s,C_s,C_{3v})$ $HCOOCH_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$HC^{12}O^{16}O^{16}C^{12}H_3$-A	C_s	501	19 985.71 M	6 914.63 M	5 304.47 M				
$HC^{12}O^{16}O^{16}C^{12}H_3$-E	C_s	502	19 980.47 M	6 913.57 M	5 304.47 M				
$DC^{12}O^{16}O^{16}C^{12}H_3$-A	C_s	503	18 479.14 M	6 768.88 M	5 109.74 M				
$DC^{12}O^{16}O^{16}C^{12}H_3$-E	C_s	504	18 474.52 M	6 768.05 M	5 109.74 M				
s-$HC^{12}O^{16}O^{16}C^{12}H_2D$-A	C_s	505	19 921.53 M	6 415.20 M	5 004.33 M				
a-$HC^{12}O^{16}O^{16}C^{12}H_2D$	C_1	506	18 517.36 M	6 729.88 M	5 165.06 M				
$HC^{12}O^{16}O^{16}C^{12}D_3$-A	C_s	507	17 261.81 M	6 101.92 M	4 778.01 M				
$HC^{13}O^{16}O^{16}C^{12}H_3$-A	C_s	508	19 802.81 M	6 865.29 M	5 262.63 M				
$HC^{13}O^{16}O^{16}C^{12}H_3$-E	C_s	509	19 798.20 M	6 864.24 M	5 262.63 M				
$HC^{12}O^{16}O^{16}C^{13}H_3$-A	C_s	511	19 769.19 M	6 743.18 M	5 188.19 M				
$HC^{12}O^{16}O^{16}C^{13}H_3$-E	C_s	512	19 764.12 M	6 742.22 M	5 188.32 M				
$HC^{12}O^{18}O^{16}C^{12}H_3$-A	C_s	513	19 529.40 M	6 617.77 M	5 097.36 M				
$HC^{12}O^{18}O^{16}C^{12}H_3$-E	C_s	514	19 525.20 M	6 616.72 M	5 097.36 M				
$HC^{12}O^{16}O^{18}C^{12}H_3$-A	C_s	515	19 326.61 M	6 849.43 M	5 219.01 M				
$HC^{12}O^{16}O^{18}C^{12}H_3$-E	C_s	516	19 322.21 M	6 848.42 M	5 219.01 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
501	1.63 M	0.68 M	0. X		1190	40					
507	1.60 M	0.76 M	0. X								

References:

ABC: 239 D_J: D_{JK}: κ: Δ:

μ: 239 eQq: V: 239 I: ω:

Coupling parameter: $I_\alpha = 3.21$ amu Å^2. Ref: 239.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$HC^{12}O^{16}O^{16}C^{12}H_3$-A	501	1, 0, 1← 0, 0, 0	Ground	A	0					12 219.29	.2	239
		1, 1, 0← 1, 0, 1	Ground	A	0					14 681.13	.2	239
		2, 0, 2← 1, 0, 1	Ground	A	0					24 298.40	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					26 048.35	.2	239
		2, 1, 2← 1, 1, 1	Ground	A	0					22 827.91	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					16 431.54	.2	239
		3, 1, 2← 3, 0, 3	Ground	A	0					19 307.57	.2	239
		3, 1, 2← 3, 1, 3	Ground	A	0					9 653.41	.35	239
		4, 1, 3← 4, 0, 4	Ground	A	0					23 562.38	.2	239
		4, 1, 3← 4, 1, 4	Ground	A	0					16 047.96	.35	239
		5, 1, 4← 5, 0, 5	Ground	A	0					29 417.37	.2	239
		5, 1, 4← 5, 1, 5	Ground	A	0					23 939.81	.35	239
		6, 2, 4← 6, 2, 5	Ground	A	0					8 577.35	.35	239
		7, 2, 5← 7, 2, 6	Ground	A	0					14 279.19	.35	239
		8, 2, 6← 8, 2, 7	Ground	A	0					21 680.87	.35	239
$HC^{12}O^{16}O^{16}C^{12}H_3$-E	502	1, 0, 1← 0, 0, 0	Ground	E	0					12 218.21	.2	239
		1, 1, 0← 1, 0, 1	Ground	E	0					14 676.59	.2	239
		2, 0, 2← 1, 0, 1	Ground	E	0					24 296.60	.2	239
		2, 1, 1← 1, 1, 0	Ground	E	0					26 044.80	.2	239
		2, 1, 1← 2, 0, 2	Ground	E	0					16 425.54	.2	239
		3, 1, 2← 3, 0, 3	Ground	E	0					19 298.88	.2	239
		3, 1, 2← 3, 1, 3	Ground	E	0					9 647.10	.35	239
		4, 1, 3← 4, 0, 4	Ground	E	0					23 550.84	.2	239
		4, 1, 3← 4, 1, 4	Ground	E	0					16 037.23	.35	239
		5, 1, 4← 5, 0, 5	Ground	E	0					29 401.50	.2	239
		5, 1, 4← 5, 1, 5	Ground	E	0					23 923.07	.35	239
		6, 2, 4← 6, 2, 5	Ground	E	0					8 571.07	.35	239
		7, 2, 5← 7, 2, 6	Ground	E	0					14 267.17	.35	239
		8, 2, 6← 8, 2, 7	Ground	E	0					21 663.10	.35	239
$DC^{12}O^{16}O^{16}C^{12}H_3$-A	503	1, 0, 1← 0, 0, 0	Ground	A	0					11 878.80	.2	239
		1, 1, 0← 1, 0, 1	Ground	A	0					13 369.38	.35	239
		2, 0, 2← 1, 0, 1	Ground	A	0					23 593.08	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					25 416.57	.2	239
		2, 1, 2← 1, 1, 1	Ground	A	0					22 097.89	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					15 192.82	.35	239
		3, 1, 2← 3, 0, 3	Ground	A	0					18 219.75	.2	239
		3, 1, 2← 3, 1, 3	Ground	A	0					9 945.74	.2	239
		4, 1, 3← 4, 0, 4	Ground	A	0					22 730.32	.2	239
		5, 1, 4← 5, 0, 5	Ground	A	0					28 936.10	.2	239
		5, 1, 4← 5, 1, 5	Ground	A	0					24 605.93	.35	239
		6, 2, 4← 6, 2, 5	Ground	A	0					9 762.83	.35	239
		7, 2, 5← 7, 2, 6	Ground	A	0					16 035.33	.35	239
		8, 2, 6← 8, 2, 7	Ground	A	0					24 027.98	.35	239
$DC^{12}O^{16}O^{16}C^{12}H_3$-E	504	1, 0, 1← 0, 0, 0	Ground	E	0					11 877.95	.2	239
		1, 1, 0← 1, 0, 1	Ground	E	0					13 365.18	.35	239
		2, 0, 2← 1, 0, 1	Ground	E	0					23 591.48	.2	239
		2, 1, 1← 1, 1, 0	Ground	E	0					25 413.66	.2	239
		2, 1, 1← 2, 0, 2	Ground	E	0					15 187.25	.2	239
		3, 1, 2← 3, 0, 3	Ground	E	0					18 212.03	.2	239

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$DC^{12}O^{16}O^{16}C^{12}H_3$-E	504	3, 1, 2← 3, 1, 3	Ground	E	0					9 939.98	.2	239
		4, 1, 3← 4, 0, 4	Ground	E	0					22 719.46	.2	239
		5, 1, 4← 5, 0, 5	Ground	E	0					29 921.44	.2	239
		5, 1, 4← 5, 1, 5	Ground	E	0					24 591.85	.35	239
		6, 2, 4← 6, 2, 5	Ground	E	0					9 756.44	.35	239
		7, 2, 5← 7, 2, 6	Ground	E	0					16 024.25	.35	239
		8, 2, 6← 8, 2, 7	Ground	E	0					24 011.56	.35	239
s-$HC^{12}O^{16}O^{16}C^{12}H_2D$-A	505	1, 0, 1← 0, 0, 0	Ground	A	0					11 419.54	.2	239
		1, 1, 0← 1, 0, 1	Ground	A	0					14 916.50	.35	239
		2, 0, 2← 1, 0, 1	Ground	A	0					22 733.95	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					24 250.27	.35	239
		2, 1, 2← 1, 1, 1	Ground	A	0					21 427.79	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					16 433.20	.2	239
		3, 1, 2← 3, 0, 3	Ground	A	0					18 896.82	.2	239
		4, 1, 3← 4, 0, 4	Ground	A	0					22 508.77	.35	239
		5, 1, 4← 5, 0, 5	Ground	A	0					27 466.07	.2	239
a-$HC^{12}O^{16}O^{16}C^{12}H_2D$	506	1, 0, 1← 0, 0, 0	Ground	A	0					11 895.09	.2	239
		1, 1, 0← 1, 0, 1	Ground	A	0					13 351.92	.35	239
		2, 0, 2← 1, 0, 1	Ground	A	0					23 644.75	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					25 354.60	.2	239
		2, 1, 2← 1, 1, 1	Ground	A	0					22 225.13	.2	239
		2, 1, 1← 2, 0, 2	Ground	E	0					15 061.90	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					15 063.28	.2	239
		5, 1, 4← 5, 0, 5	Ground	A	0					27 864.67	.2	239
		5, 1, 4← 5, 0, 5	Ground	A	0					27 868.96	.2	239
$HC^{12}O^{16}O^{16}C^{12}D_3$-A	507	1, 0, 1← 0, 0, 0	Ground	A	0					10 879.95	.2	239
		1, 1, 1← 0, 0, 0	Ground	A	0					22 039.23	.35	239
		2, 0, 2← 1, 0, 1	Ground	A	0					21 648.80	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					23 083.86	.2	239
		2, 1, 2← 1, 1, 1	Ground	A	0					20 435.80	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					13 918.67	.2	239
		3, 0, 3← 2, 1, 2	Ground	A	0					22 254.27	.35	239
		3, 1, 2← 3, 0, 3	Ground	A	0					16 270.80	.2	239
		4, 1, 3← 4, 0, 4	Ground	A	0					19 744.04	.2	239
		4, 1, 3← 4, 1, 4	Ground	A	0					13 199.17	.35	239
		5, 1, 4← 5, 0, 5	Ground	A	0					24 521.48	.2	239
		5, 1, 4← 5, 1, 5	Ground	A	0					19 697.49	.35	239
		7, 2, 5← 7, 2, 6	Ground	A	0					11 461.77	.35	239
$HC^{13}O^{16}O^{16}C^{12}H_3$-A	508	1, 0, 1← 0, 0, 0	Ground	A	0					12 127.96	.2	239
		2, 0, 2← 1, 0, 1	Ground	A	0					24 115.85	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					25 858.48	.2	239
		2, 1, 2← 1, 1, 1	Ground	A	0					22 653.03	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					16 282.62	.35	239
		3, 1, 2← 3, 0, 3	Ground	A	0					19 147.85	.2	239
		4, 1, 3← 4, 0, 4	Ground	A	0					23 388.31	.2	239
		5, 1, 4← 5, 0, 5	Ground	A	0					29 223.59	.2	239

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$HC^{13}O^{16}O^{16}C^{12}H_3$-E	509	1, 0, 1← 0, 0, 0	Ground	E	0					12 127.05	.2	239
		2, 0, 2← 1, 0, 1	Ground	E	0					24 114.02	.2	239
		2, 1, 1← 1, 1, 0	Ground	E	0					25 854.88	.2	239
		2, 1, 1← 2, 0, 2	Ground	E	0					16 276.50	.35	239
		3, 1, 2← 3, 0, 3	Ground	E	0					19 139.68	.2	239
		4, 1, 3← 4, 0, 4	Ground	E	0					23 376.87	.2	239
		5, 1, 4← 5, 0, 5	Ground	E	0					29 208.06	.2	239
$HC^{12}O^{16}O^{16}C^{13}H_3$-A	511	1, 0, 1← 0, 0, 0	Ground	A	0					11 930.69	.2	239
		2, 0, 2← 1, 0, 1	Ground	A	0					23 731.54	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					25 417.99	.2	239
		2, 1, 2← 1, 1, 1	Ground	A	0					22 307.45	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					16 266.40	.35	239
		3, 1, 2← 3, 0, 3	Ground	A	0					19 032.18	.2	239
		4, 1, 3← 4, 0, 4	Ground	A	0					23 116.71	.2	239
		5, 1, 4← 5, 0, 5	Ground	A	0					28 735.17	.2	239
$HC^{12}O^{16}O^{16}C^{13}H_3$-E	512	2, 0, 2← 1, 0, 1	Ground	E	0					23 729.67	.2	239
		2, 1, 1← 1, 1, 0	Ground	E	0					25 414.42	.2	239
		2, 1, 1← 2, 0, 2	Ground	E	0					16 260.44	.35	239
		3, 1, 2← 3, 0, 3	Ground	E	0					19 024.13	.2	239
		4, 1, 3← 4, 0, 4	Ground	E	0					23 105.61	.2	239
		5, 1, 4← 5, 0, 5	Ground	E	0					28 720.05	.2	239
$HC^{12}O^{18}O^{16}C^{12}H_3$-A	513	1, 0, 1← 0, 0, 0	Ground	A	0					11 714.45	.2	239
		2, 0, 2← 1, 0, 1	Ground	A	0					23 303.55	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					24 950.66	.2	239
		2, 1, 2← 1, 1, 1	Ground	A	0					21 909.38	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					16 078.66	.35	239
		3, 1, 2← 3, 0, 3	Ground	A	0					18 777.42	.2	239
		4, 1, 3← 4, 0, 4	Ground	A	0					22 760.03	.2	239
		5, 1, 4← 5, 0, 5	Ground	A	0					28 238.31	.2	239
$HC^{12}O^{18}O^{16}C^{12}H_3$-E	514	2, 0, 2← 1, 0, 1	Ground	E	0					23 301.71	.2	239
		2, 1, 1← 1, 1, 0	Ground	E	0					24 947.31	.2	239
		2, 1, 1← 2, 0, 2	Ground	E	0					16 073.13	.35	239
		3, 1, 2← 3, 0, 3	Ground	E	0					18 770.0	.35	239
		4, 1, 3← 4, 0, 4	Ground	E	0					22 749.66	.2	239
		5, 1, 4← 5, 0, 5	Ground	E	0					28 223.58	.35	239
$HC^{12}O^{16}O^{18}C^{12}H_3$-A	515	1, 0, 1← 0, 0, 0	Ground	A	0					12 068.35	.2	239
		2, 0, 2← 1, 0, 1	Ground	A	0					23 987.49	.2	239
		2, 1, 1← 1, 1, 0	Ground	A	0					25 767.30	.35	239
		2, 1, 2← 1, 1, 1	Ground	A	0					22 506.30	.2	239
		2, 1, 1← 2, 0, 2	Ground	A	0					15 887.28	.35	239
		3, 1, 2← 3, 0, 3	Ground	A	0					18 825.46	.2	239
		4, 1, 3← 4, 0, 4	Ground	A	0					23 185.78	.2	239
		5, 1, 4← 5, 0, 5	Ground	A	0					29 187.25	.2	239
$HC^{12}O^{16}O^{18}C^{12}H_3$-E	516	2, 0, 2← 1, 0, 1	Ground	E	0					23 985.67	.2	239
		2, 1, 1← 1, 1, 0	Ground	E	0					25 764.42	.35	239
		2, 1, 1← 2, 0, 2	Ground	E	0					15 881.96	.35	239
		3, 1, 2← 3, 0, 3	Ground	E	0					18 818.13	.35	239
		4, 1, 3← 4, 0, 4	Ground	E	0					23 174.82	.2	239
		5, 1, 4← 5, 0, 5	Ground	E	0					29 171.96	.2	239

C_2H_5Br $C_s(C_{3v},C_s)$ CH_3CH_2Br

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2Br^{79}$	C_s	521	29 956.15 M	3 803.89 M	3 522.93 M			−.9805	14.9
$C^{12}H_3C^{12}H_2Br^{81}$	C_s	522	29 947.74 M	3 781.04 M	3 503.18 M			−.9697	
$C^{12}D_3C^{12}H_2Br^{79}$	C_s	523	24 664.76 M	3 297.80 M	3 076.22 M				
$C^{12}H_3C^{12}D_2Br^{79}$	C_s	524	23 213.50 M	3 675.63 M	3 373.57 M				
$C^{12}D_3C^{12}H_2Br^{81}$	C_s	525	24 658.36 M	3 276.93 M	3 057.95 M				
$C^{12}H_3C^{12}D_2Br^{81}$	C_s	526	23 207.08 M	3 652.69 M	3 354.07 M				
$C^{12}H_3C^{13}H_2Br^{79}$	C_s	527	29 147.7 M	3 765.51 M	3 478.75 M				
$C^{13}H_3C^{12}H_2Br^{79}$	C_s	528	29 665.0 M	3 669.97 M	3 403.97 M				
$C^{12}H_3C^{13}H_2Br^{81}$	C_s	529	29 124.7 M	3 742.39 M	3 458.83 M				
$C^{13}H_3C^{12}H_2Br^{81}$	C_s	531	29 659.1 M	3 647.37 M	3 384.41 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
521	2.03 T		0. X	537.5	3567	30	5.11				
522				450.9							

References:

ABC: 361 D_J: D_{JK}: κ: 197 Δ: 253

μ: 393 eQq: 197 V: 253 I: 124 ω:

Add. Refs.: 50, 269

Torsional frequency = 202 cm^{-1}. Ref: 197.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2Br^{79}$	521	3, 0, 3← 2, 0, 2	Ground				9/2		7/2	21 966.25	.05	361
		3, 0, 3← 2, 0, 2	Ground				7/2		5/2	21 966.25	.05	361
		3, 0, 3← 2, 0, 2	Ground							21 972.6		124
		3, 0, 3← 2, 0, 2	Ground				3/2		1/2	21 991.60	.05	361
		3, 0, 3← 2, 0, 2	Ground				5/2		3/2	21 992.44	.05	361
		3, 1, 2← 2, 1, 1	Ground				3/2		1/2	22 386.74	.05	361
		3, 1, 2← 2, 1, 1	Ground				9/2		7/2	22 388.13	.05	361
		3, 1, 2← 2, 1, 1	Ground				5/2		3/2	22 409.10	.05	361
		3, 1, 2← 2, 1, 1	Ground				7/2		5/2	22 415.50	.05	361
		3, 1, 3← 2, 1, 2	Ground				9/2		7/2	21 545.67	.05	361
		3, 1, 3← 2, 1, 2	Ground				3/2		1/2	21 550.04	.05	361
		3, 1, 3← 2, 1, 2	Ground							21 557.2		197
		3, 1, 3← 2, 1, 2	Ground				7/2		5/2	21 571.56	.05	361
		3, 1, 3← 2, 1, 2	Ground				5/2		3/2	21 576.45	.05	361
		3, 2, 1← 2, 2, 0	Ground				3/2		1/2	21 885.70		197
		3, 2, 1← 2, 2, 0	Ground	E	1		9/2		7/2	21 903.41	.10	253
		3, 2, 1← 2, 2, 0	Ground	A	1		9/2		7/2	21 905.25	.10	253
		3, 2, 1← 2, 2, 0	Ground				9/2		7/2	21 959.77		197
		3, 2, 1← 2, 2, 0	Ground							21 989.7		197
		3, 2, 1← 2, 2, 0	Ground				5/2		3/2	21 990.15		197
		3, 2, 1← 2, 2, 0	Ground	E	1		7/2		5/2	22 007.57	.10	253
		3, 2, 1← 2, 2, 0	Ground	A	1		7/2		5/2	22 009.50	.10	253
		3, 2, 1← 2, 2, 0	Ground				7/2		5/2	22 064.16		197
		3, 2, 2← 2, 2, 1	Ground				3/2		1/2	21 876.90		197
		3, 2, 2← 2, 2, 1	Ground	A	1		9/2		7/2	21 896.58	.10	253
		3, 2, 2← 2, 2, 1	Ground	E	1		9/2		7/2	21 898.43	.10	253
		3, 2, 2← 2, 2, 1	Ground				9/2		7/2	21 951.20		197
		3, 2, 2← 2, 2, 1	Ground							21 981.1		197
		3, 2, 2← 2, 2, 1	Ground				5/2		3/2	21 981.20		197
		3, 2, 2← 2, 2, 1	Ground	A	1		7/2		5/2	22 001.05	.10	253
		3, 2, 2← 2, 2, 1	Ground	E	1		7/2		5/2	22 002.99	.01	253
		3, 2, 2← 2, 2, 1	Ground				7/2		5/2	22 055.60		197
		4, 1, 4← 3, 1, 3	Ground				11/2		9/2	28 733.50		197
		4, 1, 4← 3, 1, 3	Ground							28 740.1		197
		4, 1, 4← 3, 1, 3	Ground				5/2		3/2	28 740.80		197
		4, 1, 4← 3, 1, 3	Ground				9/2		7/2	28 743.80		197
		4, 1, 4← 3, 1, 3	Ground				7/2		5/2	28 751.00		197
		4, 2, 2← 3, 2, 1	Ground	E	1		7/2		5/2	29 265.88	.01	253
		4, 2, 2← 3, 2, 1	Ground	A	1		7/2		5/2	29 266.88	.01	253
		4, 2, 3← 3, 2, 2	Ground	A	1		11/2		9/2	29 217.71	.01	253
		4, 2, 3← 3, 2, 2	Ground	E	1		11/2		9/2	29 218.71	.01	253
		4, 2, 3← 3, 2, 2	Ground	A	1		9/2		7/2	29 259.34	.01	253
		4, 2, 3← 3, 2, 2	Ground	E	1		9/2		7/2	29 260.47	.01	253
		5, 1, 4← 5, 0, 5	Ground				13/2		11/2	28 445.75	.05	361
		5, 1, 4← 5, 0, 5	Ground				11/2		9/2	28 453.58	.05	361
		5, 1, 4← 5, 0, 5	Ground				15/2		13/2	28 473.63	.05	361
		5, 1, 4← 5, 0, 5	Ground				9/2		7/2	28 480.95	.05	361
		7, 1, 6← 7, 0, 7	Ground				17/2		15/2	30 431.79	.05	361
		7, 1, 6← 7, 0, 7	Ground				15/2		13/2	30 436.59	.05	361
		7, 1, 6← 7, 0, 7	Ground				19/2		17/2	30 455.39	.05	361

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2Br^{79}$	521	7, 1, 6← 7, 0, 7	Ground				13/2		11/2	30 460.07	.05	361
$C^{12}H_3C^{12}H_2Br^{81}$	522	3, 0, 3← 2, 0, 2	Ground				7/2		5/2	21 839.67	.05	361
		3, 0, 3← 2, 0, 2	Ground				9/2		7/2	21 839.67	.05	361
		3, 0, 3← 2, 0, 2	Ground				3/2		1/2	21 860.97	.05	361
		3, 0, 3← 2, 0, 2	Ground				5/2		3/2	21 861.55	.05	361
		3, 1, 2← 2, 1, 1	Ground				3/2		1/2	22 256.63	.05	361
		3, 1, 2← 2, 1, 1	Ground				9/2		7/2	22 258.07	.05	361
		3, 1, 2← 2, 1, 1	Ground				5/2		3/2	22 275.75	.05	361
		3, 1, 2← 2, 1, 1	Ground				7/2		5/2	22 280.80	.05	361
		3, 1, 3← 2, 1, 2	Ground				9/2		7/2	21 424.66	.05	361
		3, 1, 3← 2, 1, 2	Ground				3/2		1/2	21 428.29	.05	361
		3, 1, 3← 2, 1, 2	Ground							21 434.1		197
		3, 1, 3← 2, 1, 2	Ground				7/2		5/2	21 446.41	.05	361
		3, 1, 3← 2, 1, 2	Ground				5/2		3/2	21 450.32	.05	361
		3, 2, 1← 2, 2, 0	Ground				3/2		1/2	21 774.92		197
		3, 2, 1← 2, 2, 0	Ground	E	1		9/2		7/2	21 780.69	.01	253
		3, 2, 1← 2, 2, 0	Ground	A	1		9/2		7/2	21 782.67	.01	253
		3, 2, 1← 2, 2, 0	Ground				9/2		7/2	21 837.10		197
		3, 2, 1← 2, 2, 0	Ground							21 862.0		197
		3, 2, 1← 2, 2, 0	Ground				5/2		3/2	21 862.13		197
		3, 2, 1← 2, 2, 0	Ground	E	1		7/2		5/2	21 867.70	.01	253
		3, 2, 1← 2, 2, 0	Ground	A	1		7/2		5/2	21 869.65	.01	253
		3, 2, 1← 2, 2, 0	Ground				7/2		5/2	21 924.14		197
		3, 2, 2← 2, 2, 1	Ground				9/2		7/2	21 828.23		197
		3, 2, 2← 2, 2, 1	Ground							21 853.3		197
		3, 2, 2← 2, 2, 1	Ground				5/2		3/2	21 853.46		197
		3, 2, 2← 2, 2, 1	Ground				7/2		5/2	21 915.73		197
		4, 1, 4← 3, 1, 3	Ground				11/2		9/2	28 570.80		197
		4, 1, 4← 3, 1, 3	Ground							28 576.3		197
		4, 1, 4← 3, 1, 3	Ground				5/2		3/2	28 576.70		197
		4, 1, 4← 3, 1, 3	Ground				9/2		7/2	28 579.50		197
		4, 1, 4← 3, 1, 3	Ground				7/2		5/2	28 585.70		197
		4, 2, 3← 3, 2, 2	Ground	A	1		9/2		7/2	29 093.65	.01	253
		4, 2, 3← 3, 2, 2	Ground	E	1		9/2		7/2	29 094.66	.01	253
		5, 1, 4← 5, 0, 5	Ground				11/2		11/2	28 436.96	.05	361
		5, 1, 4← 5, 0, 5	Ground				9/2		9/2	28 443.22	.05	361
		5, 1, 4← 5, 0, 5	Ground				13/2		13/2	28 460.03	.05	361
		5, 1, 4← 5, 0, 5	Ground				7/2		7/2	28 466.19	.05	361
		7, 1, 6← 7, 0, 7	Ground				15/2		15/2	30 398.44	.05	361
		7, 1, 6← 7, 0, 7	Ground				13/2		13/2	30 402.48	.05	361
		7, 1, 6← 7, 0, 7	Ground				17/2		17/2	30 418.10	.05	361
		7, 1, 6← 7, 0, 7	Ground				11/2		11/2	30 422.02	.05	361
$C^{12}D_3C^{12}H_2Br^{79}$	523	3, 0, 3← 2, 0, 2	Ground				7/2		5/2	19 109.86	.05	361
		3, 0, 3← 2, 0, 2	Ground				9/2		7/2	19 110.67	.05	361
		3, 0, 3← 2, 0, 2	Ground				3/2		1/2	19 133.69	.05	361
		3, 0, 3← 2, 0, 2	Ground				5/2		3/2	19 135.33	.05	361
		3, 1, 2← 2, 1, 1	Ground				3/2		1/2	19 439.72	.05	361

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3C^{12}H_2Br^{79}$	523	3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	19 441.68	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	19 460.56	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	19 467.83	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	18 777.32	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	18 782.26	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	18 801.98	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	18 807.27	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			13/2		13/2	23 881.79	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			11/2		11/2	23 888.35	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			15/2		15/2	23 909.10	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			9/2		9/2	23 915.29	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			15/2		15/2	24 731.52	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			13/2		13/2	24 736.91	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			17/2		17/2	24 757.70	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			11/2		11/2	24 762.80	.05	361
$C^{12}H_3C^{12}D_2Br^{79}$	524	3, 0, 3 ← 2, 0, 2	Ground			9/2		7/2	21 128.81	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			7/2		5/2	21 132.01	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			5/2		3/2	21 157.81	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			3/2		1/2	21 162.20	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			3/2		1/2	21 584.83	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	21 590.35	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	21 616.46	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	21 617.29	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	20 680.26	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	20 684.07	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	20 707.16	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	20 711.43	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			11/2		11/2	22 035.23	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			9/2		9/2	22 042.53	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			13/2		13/2	22 061.39	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			7/2		7/2	22 068.60	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			13/2		13/2	23 036.91	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			11/2		11/2	23 041.97	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			15/2		15/2	23 060.18	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			9/2		9/2	23 065.47	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			15/2		15/2	24 240.94	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			13/2		13/2	24 245.82	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			17/2		17/2	24 263.26	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			11/2		11/2	24 267.19	.05	361
$C^{12}D_3C^{12}H_2Br^{81}$	525	3, 0, 3 ← 2, 0, 2	Ground			7/2		5/2	18 993.67	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			9/2		7/2	18 994.08	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			3/2		1/2	19 013.66	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			5/2		3/2	19 014.75	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			3/2		1/2	19 320.66	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	19 322.63	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	19 338.73	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	19 344.35	.05	361

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3C^{12}H_2Br^{81}$	525	3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	18 665.63	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	18 669.75	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	18 686.28	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	18 690.79	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			13/2		13/2	23 868.13	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			11/2		11/2	23 873.61	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			15/2		15/2	23 890.79	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			9/2		9/2	23 896.07	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			15/2		15/2	24 706.90	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			13/2		13/2	24 711.31	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			17/2		17/2	24 728.53	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			11/2		11/2	24 731.62	.05	361
$C^{12}H_3C^{12}D_2Br^{81}$	526	3, 0, 3 ← 2, 0, 2	Ground			9/2		7/2	21 002.59	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			7/2		5/2	21 005.19	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			5/2		3/2	21 026.68	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			3/2		1/2	21 030.18	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			3/2		1/2	21 454.68	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	21 459.19	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	21 481.07	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	21 481.74	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	20 560.17	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	20 563.36	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	20 582.64	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	20 586.21	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			11/2		11/2	22 024.46	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			9/2		9/2	22 030.70	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			13/2		13/2	22 046.34	.05	361
		5, 1, 4 ← 5, 0, 5	Ground			7/2		7/2	22 052.26	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			13/2		13/2	23 012.88	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			11/2		11/2	23 017.24	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			15/2		15/2	23 032.66	.05	361
		6, 1, 5 ← 6, 0, 6	Ground			9/2		9/2	23 036.91	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			15/2		15/2	24 201.97	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			13/2		13/2	24 205.84	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			17/2		17/2	24 220.70	.05	361
		7, 1, 6 ← 7, 0, 7	Ground			11/2		11/2	24 224.11	.05	361
$C^{12}H_3C^{13}H_2Br^{79}$	527	3, 0, 3 ← 2, 0, 2	Ground			9/2		7/2	21 718.20	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			5/2		3/2	21 744.70	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			3/2		1/2	22 147.69	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	22 149.41	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	22 170.88	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	22 176.84	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	21 289.31	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	21 293.52	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	21 315.48	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	21 320.07	.05	361

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_3C^{12}H_2Br^{79}$	528	3, 0, 3 ← 2, 0, 2	Ground			9/2		7/2	21 208.90	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			5/2		3/2	21 233.95	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			3/2		1/2	21 605.90	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	21 606.77	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	21 626.46	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	21 634.34	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	20 809.94	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	20 814.35	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	20 835.57	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	20 840.44	.05	361
$C^{12}H_3C^{13}H_2Br^{81}$	529	3, 0, 3 ← 2, 0, 2	Ground			9/2		7/2	21 590.10	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			5/2		3/2	21 612.01	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			3/2		1/2	22 016.12	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	22 017.62	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	22 035.68	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	22 040.21	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	21 166.97	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	21 170.52	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	21 188.89	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	21 192.78	.05	361
$C^{13}H_3C^{12}H_2Br^{81}$	531	3, 0, 3 ← 2, 0, 2	Ground			9/2		7/2	21 083.35	.05	361
		3, 0, 3 ← 2, 0, 2	Ground			5/2		3/2	21 104.47	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			9/2		7/2	21 447.98	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			5/2		3/2	21 494.67	.05	361
		3, 1, 2 ← 2, 1, 1	Ground			7/2		5/2	21 501.20	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			9/2		7/2	20 689.88	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			3/2		1/2	20 693.57	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			7/2		5/2	20 711.40	.05	361
		3, 1, 3 ← 2, 1, 2	Ground			5/2		3/2	20 715.41	.05	361

C_2H_5Cl $C_s(C_{3v},C_s)$ CH_3CH_2Cl

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2Cl^{35}$	C_s	541	31 337.35 M	5 493.69 M	4 962.30 M				18.9
$C^{12}H_3C^{12}H_2Cl^{37}$	C_s	542	31 285.20 M	5 378.99 M	4 867.23 M				
t-$C^{12}H_2DC^{12}H_2Cl^{35}$	C_s	543	31 293.39 M	5 098.65 M	4 637.60 M				
g-$C^{12}H_2DC^{12}H_2Cl^{35}$	C_1	544	28 307.27 M	5 297.52 M	4 784.93 M				
$C^{13}H_3C^{12}H_2Cl^{35}$	C_s	545	31 081.22 M	5 325.59 M	4 818.56 M				
$C^{12}H_3C^{13}H_2Cl^{35}$	C_s	546	30 523.34 M	5 472.41 M	4 923.99 M				
$C^{12}H_3C^{12}D_2Cl^{35}$	C_s	547	24 140.20 M	5 352.75 M	4 772.09 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
541	1.79 M		0. X	−49.20	3560	12		336 1			
542				−38.65							
543				−49.32							
544				−47.36							
545				−48.48							
546				−49.51							
547				−51.07							

References:

ABC: 196, 357 D_J: D_{JK}: κ: Δ: 253

μ: 127 eQq: 357 V: 253 I: ω: 253

Torsional frequency = 242.5 cm^{-1}. Ref: 253.
Coupling Parameter: $I_\alpha = 3.1613$ amu Å^2. Ref: 357.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2Cl^{35}$	541	1, 0, 1← 0, 0, 0	Ground				3/2		3/2	10 446.11	.05	357
		1, 0, 1← 0, 0, 0	Ground							10 456.00	.05	357
		1, 0, 1← 0, 0, 0	Ground				5/2		3/2	10 458.46	.05	357
		1, 0, 1← 0, 0, 0	Ground				1/2		3/2	10 468.37	.05	357
		2, 0, 2← 1, 0, 1	Ground				3/2		1/2	20 891.45	.05	357
		2, 0, 2← 1, 0, 1	Ground				5/2		5/2	20 892.41	.05	357
		2, 0, 2← 1, 0, 1	Ground							20 903.77	.05	357
		2, 0, 2← 1, 0, 1	Ground				5/2		3/2	20 904.87	.05	357
		2, 0, 2← 1, 0, 1	Ground				7/2		5/2	20 904.87	.05	357
		2, 0, 2← 1, 0, 1	Ground				3/2		3/2	20 913.69	.05	357
		2, 1, 1← 1, 1, 0	Ground	A	1		5/2		3/2	21 376.08	.1	196
		2, 1, 1← 1, 1, 0	Ground	A	1		3/2		3/2	21 378.65	.1	196
		2, 1, 1← 1, 1, 0	Ground	A	1		5/2		5/2	21 385.02	.1	196
		2, 1, 1← 1, 1, 0	Ground	A	1		7/2		5/2	21 388.49	.1	196
		2, 1, 1← 1, 1, 0	Ground	A	1		3/2		1/2	21 394.83	.1	196
		2, 1, 1← 1, 1, 0	Ground	A	1		1/2		1/2	21 398.18	.1	196
		2, 1, 1← 1, 1, 0	Ground				5/2		3/2	21 433.79	.05	357
		2, 1, 1← 1, 1, 0	Ground				3/2		3/2	21 436.27	.05	357
		2, 1, 1← 1, 1, 0	Ground				5/2		5/2	21 442.73	.05	357
		2, 1, 1← 1, 1, 0	Ground							21 443.38	.05	357
		2, 1, 1← 1, 1, 0	Ground				7/2		5/2	21 446.21	.05	357
		2, 1, 1← 1, 1, 0	Ground				3/2		1/2	21 452.27	.05	357
		2, 1, 1← 1, 1, 0	Ground				1/2		1/2	21 455.62	.05	357
		2, 1, 2← 1, 1, 1	Ground				5/2		3/2	20 371.50	.05	357
		2, 1, 2← 1, 1, 1	Ground				5/2		5/2	20 374.88	.05	357
		2, 1, 2← 1, 1, 1	Ground				3/2		3/2	20 377.89	.05	357
		2, 1, 2← 1, 1, 1	Ground							20 380.58	.05	357
		2, 1, 2← 1, 1, 1	Ground				7/2		5/2	20 383.79	.05	357
		2, 1, 2← 1, 1, 1	Ground				1/2		1/2	20 392.86	.05	357
		3, 2, 1← 2, 2, 0	Ground	E	1		7/2		5/2	31 311.95	.10	253
		3, 2, 1← 2, 2, 0	Ground	A	1		7/2		5/2	31 314.48	.10	253
		3, 2, 1← 2, 2, 0	Ground	E	1		5/2		3/2	31 320.82	.10	253
		3, 2, 1← 2, 2, 0	Ground	A	1		5/2		3/2	31 323.36	.10	253
		3, 2, 1← 2, 2, 0	Ground	E	1		9/2		7/2	31 324.37	.10	253
		3, 2, 1← 2, 2, 0	Ground	A	1		9/2		7/2	31 326.78	.10	253
		3, 2, 1← 2, 2, 0	Ground	E	1		3/2		1/2	31 333.03	.10	253
		3, 2, 1← 2, 2, 0	Ground	A	1		3/2		1/2	31 335.62	.10	253
		3, 2, 1← 2, 2, 0	1				7/2		5/2	31 345.78	.10	253
		3, 2, 1← 2, 2, 0	1				5/2		3/2	31 354.66	.10	253
		3, 2, 1← 2, 2, 0	Ground				7/2		5/2	31 391.53	.1	196
		3, 2, 1← 2, 2, 0	Ground							31 400.29	.1	196
		3, 2, 1← 2, 2, 0	Ground				5/2		3/2	31 400.44	.1	196
		3, 2, 1← 2, 2, 0	Ground				9/2		7/2	31 403.78	.1	196
		3, 2, 1← 2, 2, 0	Ground				3/2		1/2	31 412.5	.1	196
		3, 2, 2← 2, 2, 1	Ground	A	1		7/2		5/2	31 282.66	.10	253
		3, 2, 2← 2, 2, 1	Ground	E	1		7/2		5/2	31 285.27	.10	253
		3, 2, 2← 2, 2, 1	Ground	A	0		5/2		3/2	31 291.62	.10	253
		3, 2, 2← 2, 2, 1	Ground	E	0		5/2		3/2	31 294.25	.10	253
		3, 2, 2← 2, 2, 1	Ground	A	1		9/2		7/2	31 295.17	.10	253
		3, 2, 2← 2, 2, 1	Ground	E	1		9/2		7/2	31 297.67	.10	253

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2Cl^{35}$	541	3, 2, 2← 2, 2, 1	Ground	A 1		3/2		1/2	31 303.94	.10	253
		3, 2, 2← 2, 2, 1	Ground	E 1		3/2		1/2	31 306.46	.10	253
		3, 2, 2← 2, 2, 1	1			7/2		5/2	31 312.97	.10	253
		3, 2, 2← 2, 2, 1	1			5/2		3/2	31 321.86	.10	253
		3, 2, 2← 2, 2, 1	1			9/2		7/2	31 325.49	.10	253
		3, 2, 2← 2, 2, 1	1			3/2		1/2	31 333.95	.10	253
		3, 2, 2← 2, 2, 1	Ground			7/2		5/2	31 359.15	.1	196
		3, 2, 2← 2, 2, 1	Ground			5/2		3/2	31 367.95	.1	196
		3, 2, 2← 2, 2, 1	Ground						31 368.07	.1	196
		3, 2, 2← 2, 2, 1	Ground			9/2		7/2	31 371.65	.1	196
		3, 2, 2← 2, 2, 1	Ground			3/2		1/2	31 380.55	.1	196
		3, 1, 2← 3, 0, 3	Ground			3/2		3/2	27 734.22	.05	357
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	27 737.03	.05	357
		3, 1, 2← 3, 0, 3	Ground			5/2		5/2	27 740.18	.05	357
		3, 1, 2← 3, 0, 3	Ground			7/2		7/2	27 742.95	.05	357
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	28 862.92	.05	357
		4, 1, 3← 4, 0, 4	Ground			11/2		11/2	28 864.73	.05	357
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	28 867.92	.05	357
		4, 1, 3← 4, 0, 4	Ground			9/2		9/2	28 869.63	.05	357
		5, 0, 5← 4, 1, 4	Ground						28 563.29	.05	357
$C^{12}H_3C^{12}H_2Cl^{37}$	542	1, 0, 1← 0, 0, 0	Ground			3/2		3/2	10 238.66	.05	324
		1, 0, 1← 0, 0, 0	Ground			5/2		3/2	10 248.08	.05	324
		1, 0, 1← 0, 0, 0	Ground			1/2		3/2	10 255.97	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		3/2	20 996.90	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		3/2	20 998.48	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		5/2	21 003.51	.05	324
		2, 1, 1← 1, 1, 0	Ground			7/2		5/2	21 006.28	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		1/2	21 011.02	.05	324
		2, 1, 1← 1, 1, 0	Ground			1/2		1/2	21 013.94	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		3/2	19 973.43	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		5/2	19 976.16	.05	324
		2, 1, 2← 1, 1, 1	Ground			3/2		3/2	19 978.51	.05	324
		2, 1, 2← 1, 1, 1	Ground			7/2		5/2	19 983.22	.05	324
		2, 1, 2← 1, 1, 1	Ground			1/2		1/2	19 990.44	.05	324
		3, 1, 2← 3, 0, 3	Ground			3/2		3/2	27 726.70	.05	324
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	27 728.65	.05	324
		3, 1, 2← 3, 0, 3	Ground			5/2		5/2	27 730.75	.05	324
		3, 1, 2← 3, 0, 3	Ground			7/2		7/2	27 733.35	.05	324
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	28 810.74	.05	324
		4, 1, 3← 4, 0, 4	Ground			11/2		11/2	28 812.06	.05	324
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	28 814.56	.05	324
		4, 1, 3← 4, 0, 4	Ground			9/2		9/2	28 815.92	.05	324
		5, 0, 5← 4, 1, 4	Ground						27 382.99	.05	357
		5, 1, 4← 5, 0, 5	Ground			7/2		7/2	30 206.62	.05	324
		5, 1, 4← 5, 0, 5	Ground			13/2		13/2	30 207.53	.05	324
		5, 1, 4← 5, 0, 5	Ground			9/2		9/2	30 209.95	.05	324
		5, 1, 4← 5, 0, 5	Ground			11/2		11/2	30 210.87	.05	324

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
t-$C^{12}H_2DC^{12}H_2Cl^{35}$	543	1, 0, 1← 0, 0, 0	Ground			3/2		3/2	9 726.45	.05	324
		1, 0, 1← 0, 0, 0	Ground			5/2		3/2	9 738.77	.05	324
		1, 0, 1← 0, 0, 0	Ground			1/2		3/2	9 748.59	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		3/2	19 923.90	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		3/2	19 926.35	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		5/2	19 932.95	.05	324
		2, 1, 1← 1, 1, 0	Ground			7/2		5/2	19 936.20	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		1/2	19 942.45	.05	324
		2, 1, 1← 1, 1, 0	Ground			1/2		1/2	19 945.95	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		3/2	19 002.3	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		5/2	19 005.8	.05	324
		2, 1, 2← 1, 1, 1	Ground			3/2		3/2	19 008.6	.05	324
		2, 1, 2← 1, 1, 1	Ground			7/2		5/2	19 014.6	.05	324
		2, 1, 2← 1, 1, 1	Ground			1/2		1/2	19 023.9	.05	324
		3, 2, 1← 2, 2, 0	Ground			7/2		5/2	29 224.23	.1	196
		3, 2, 1← 2, 2, 0	Ground			5/2		3/2	29 233.08	.1	196
		3, 2, 1← 2, 2, 0	Ground			9/2		7/2	29 236.53	.1	196
		3, 2, 1← 2, 2, 0	Ground			3/2		1/2	29 245.64	.1	196
		3, 2, 2← 2, 2, 1	Ground			7/2		5/2	29 200.14	.1	196
		3, 2, 2← 2, 2, 1	Ground			5/2		3/2	29 208.89	.1	196
		3, 2, 2← 2, 2, 1	Ground			9/2		7/2	29 212.44	.1	196
		3, 1, 2← 3, 0, 3	Ground			3/2		3/2	27 830.10	.05	324
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	27 832.83	.05	324
		3, 1, 2← 3, 0, 3	Ground			5/2		5/2	27 835.97	.05	324
		3, 1, 2← 3, 0, 3	Ground			7/2		7/2	27 838.62	.05	324
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	28 801.67	.05	324
		4, 1, 3← 4, 0, 4	Ground			11/2		11/2	28 803.29	.05	324
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	28 806.52	.05	324
		4, 1, 3← 4, 0, 4	Ground			9/2		9/2	28 808.10	.05	324
		5, 0, 5← 4, 1, 4	Ground						24 368.57	.05	357
		5, 1, 4← 5, 0, 5	Ground			7/2		7/2	30 048.54	.05	324
		5, 1, 4← 5, 0, 5	Ground			13/2		13/2	30 049.65	.05	324
		5, 1, 4← 5, 0, 5	Ground			9/2		9/2	30 052.73	.05	324
		5, 1, 4← 5, 0, 5	Ground			11/2		11/2	30 053.86	.05	324
g-$C^{12}H_2DC^{12}H_2Cl^{35}$	544	1, 0, 1← 0, 0, 0	Ground			3/2		3/2	10 072.98	.05	324
		1, 0, 1← 0, 0, 0	Ground			5/2		3/2	10 084.92	.05	324
		1, 0, 1← 0, 0, 0	Ground			1/2		3/2	10 094.21	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		3/2	20 668.28	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		3/2	20 670.34	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		5/2	20 677.17	.05	324
		2, 1, 1← 1, 1, 0	Ground			7/2		5/2	20 680.09	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		1/2	20 686.34	.05	324
		2, 1, 1← 1, 1, 0	Ground			1/2		1/2	20 689.31	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		3/2	19 643.6	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		5/2	19 646.4	.05	324
		2, 1, 2← 1, 1, 1	Ground			3/2		3/2	19 650.0	.05	324
		2, 1, 2← 1, 1, 1	Ground			7/2		5/2	19 655.4	.05	324
		2, 1, 2← 1, 1, 1	Ground			1/2		1/2	19 664.2	.05	324
		3, 2, 1← 2, 2, 0	Ground			7/2		5/2	30 272.84	.1	196
		3, 2, 1← 2, 2, 0	Ground			5/2		3/2	30 281.45	.1	196

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
g-$C^{12}H_2DC^{12}H_2Cl^{35}$	544	3, 2, 1← 2, 2, 0	Ground			9/2		7/2	30 284.50	.1	196
		3, 2, 1← 2, 2, 0	Ground			3/2		1/2	30 293.03	.1	196
		3, 2, 2← 2, 2, 1	Ground			7/2		5/2	30 238.96	.1	196
		3, 2, 2← 2, 2, 1	Ground			5/2		3/2	30 247.36	.1	196
		3, 2, 2← 2, 2, 1	Ground			9/2		7/2	30 250.87	.1	196
		3, 2, 2← 2, 2, 1	Ground			3/2		1/2	30 259.08	.1	196
		3, 1, 2← 3, 0, 3	Ground			3/2		3/2	24 835.97	.05	324
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	24 838.76	.05	324
		3, 1, 2← 3, 0, 3	Ground			5/2		5/2	24 842.03	.05	324
		3, 1, 2← 3, 0, 3	Ground			7/2		7/2	24 844.87	.05	324
		5, 0, 5← 4, 1, 4	Ground						29 433.82	.05	357
		5, 1, 4← 5, 0, 5	Ground			7/2		7/2	27 342.62	.05	324
		5, 1, 4← 5, 0, 5	Ground			13/2		13/2	27 343.98	.05	324
		5, 1, 4← 5, 0, 5	Ground			9/2		9/2	27 347.22	.05	324
		5, 1, 4← 5, 0, 5	Ground			11/2		11/2	27 348.50	.05	324
		6, 1, 5← 6, 0, 6	Ground			9/2		9/2	29 104.23	.05	324
		6, 1, 5← 6, 0, 6	Ground			15/2		15/2	29 105.22	.05	324
		6, 1, 5← 6, 0, 6	Ground			11/2		11/2	29 108.62	.05	324
		6, 1, 5← 6, 0, 6	Ground			13/2		13/2	29 109.55	.05	324
$C^{13}H_3C^{12}H_2Cl^{35}$	545	2, 0, 2← 1, 0, 1	Ground			5/2		3/2	20 313.27	.05	324
		2, 0, 2← 1, 0, 1	Ground			7/2		5/2	20 315.02	.05	324
		2, 0, 2← 1, 0, 1	Ground			3/2		3/2	20 322.10	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		3/2	20 785.85	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		5/2	20 794.83	.05	324
		2, 1, 1← 1, 1, 0	Ground			7/2		5/2	20 798.02	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		1/2	20 804.15	.05	324
		2, 1, 1← 1, 1, 0	Ground			1/2		1/2	20 807.44	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		3/2	19 772.27	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		5/2	19 775.61	.05	324
		2, 1, 2← 1, 1, 1	Ground			3/2		3/2	19 778.66	.05	324
		2, 1, 2← 1, 1, 1	Ground			7/2		5/2	19 784.42	.05	324
		2, 1, 2← 1, 1, 1	Ground			1/2		1/2	19 793.4	.05	324
		3, 1, 2← 3, 0, 3	Ground			3/2		3/2	27 557.89	.05	324
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	27 560.62	.05	324
		3, 1, 2← 3, 0, 3	Ground			5/2		5/2	27 563.76	.05	324
		3, 1, 2← 3, 0, 3	Ground			7/2		7/2	27 566.63	.05	324
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	28 632.35	.05	324
		4, 1, 3← 4, 0, 4	Ground			11/2		11/2	28 634.10	.05	324
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	28 637.11	.05	324
		4, 1, 3← 4, 0, 4	Ground			9/2		9/2	28 638.88	.05	324
		5, 1, 4← 5, 0, 5	Ground			7/2		7/2	30 015.11	.05	324
		5, 1, 4← 5, 0, 5	Ground			13/2		13/2	30 016.32	.05	324
		5, 1, 4← 5, 0, 5	Ground			9/2		9/2	30 019.42	.05	324
		5, 1, 4← 5, 0, 5	Ground			11/2		11/2	30 020.68	.05	324
$C^{12}H_3C^{13}H_2Cl^{35}$	546	1, 0, 1← 0, 0, 0	Ground			3/2		3/2	10 386.51	.05	324
		1, 0, 1← 0, 0, 0	Ground			5/2		3/2	10 398.86	.05	324
		1, 0, 1← 0, 0, 0	Ground			1/2		3/2	10 408.78	.05	324
		2, 0, 2← 1, 0, 1	Ground			3/2		1/2	20 771.41	.05	324
		2, 0, 2← 1, 0, 1	Ground			5/2		5/2	20 772.35	.05	324
		2, 0, 2← 1, 0, 1	Ground			7/2		5/2	20 784.91	.05	324

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{13}H_2Cl^{35}$	546	2, 0, 2← 1, 0, 1	Ground			3/2		3/2	20 793.67	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		3/2	21 331.72	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		3/2	21 334.11	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		5/2	21 340.42	.05	324
		2, 1, 1← 1, 1, 0	Ground			7/2		5/2	21 344.00	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		1/2	21 349.93	.05	324
		2, 1, 1← 1, 1, 0	Ground			1/2		1/2	21 353.66	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		3/2	20 235.21	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		5/2	20 238.71	.05	324
		2, 1, 2← 1, 1, 1	Ground			3/2		3/2	20 241.57	.05	324
		2, 1, 2← 1, 1, 1	Ground			7/2		5/2	20 247.70	.05	324
		2, 1, 2← 1, 1, 1	Ground			1/2		1/2	20 256.75	.05	324
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	28 173.62	.05	324
		4, 1, 3← 4, 0, 4	Ground			11/2		11/2	28 175.25	.05	324
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	28 178.26	.05	324
		4, 1, 3← 4, 0, 4	Ground			9/2		9/2	28 179.95	.05	324
		5, 0, 5← 4, 1, 4	Ground						29 109.25	.05	357
		5, 1, 4← 5, 0, 5	Ground			7/2		7/2	29 682.75	.05	324
		5, 1, 4← 5, 0, 5	Ground			13/2		13/2	29 683.97	.05	324
		5, 1, 4← 5, 0, 5	Ground			9/2		9/2	29 686.99	.05	324
		5, 1, 4← 5, 0, 5	Ground			11/2		11/2	29 688.18	.05	324
$C^{12}H_3C^{12}D_2Cl^{35}$	547	2, 0, 2← 1, 0, 1	Ground			3/2		1/2	20 223.65	.05	324
		2, 0, 2← 1, 0, 1	Ground			5/2		5/2	20 224.63	.05	324
		2, 0, 2← 1, 0, 1	Ground						20 236.43	.05	357
		2, 0, 2← 1, 0, 1	Ground			5/2		3/2	20 237.46	.05	324
		2, 0, 2← 1, 0, 1	Ground			3/2		3/2	20 246.72	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		3/2	20 820.49	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		3/2	20 823.26	.05	324
		2, 1, 1← 1, 1, 0	Ground			5/2		5/2	20 829.38	.05	324
		2, 1, 1← 1, 1, 0	Ground						20 830.34	.05	357
		2, 1, 1← 1, 1, 0	Ground			7/2		5/2	20 833.26	.05	324
		2, 1, 1← 1, 1, 0	Ground			3/2		1/2	20 839.28	.05	324
		2, 1, 1← 1, 1, 0	Ground			1/2		1/2	20 843.07	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		3/2	19 659.54	.05	324
		2, 1, 2← 1, 1, 1	Ground			5/2		5/2	19 663.44	.05	324
		2, 1, 2← 1, 1, 1	Ground			3/2		3/2	19 665.87	.05	324
		2, 1, 2← 1, 1, 1	Ground						19 669.02	.05	357
		2, 1, 2← 1, 1, 1	Ground			7/2		5/2	19 672.38	.05	324
		2, 1, 2← 1, 1, 1	Ground			1/2		1/2	19 681.83	.05	324
		3, 1, 2← 3, 0, 3	Ground			3/2		3/2	20 872.9	.05	324
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	20 875.6	.05	324
		3, 1, 2← 3, 0, 3	Ground						20 877.60	.05	357
		3, 1, 2← 3, 0, 3	Ground			5/2		5/2	20 878.7	.05	324
		3, 1, 2← 3, 0, 3	Ground			7/2		7/2	20 881.6	.05	324
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	22 140.38	.05	324
		4, 1, 3← 4, 0, 4	Ground			11/2		11/2	22 142.19	.05	324
		4, 1, 3← 4, 0, 4	Ground						22 143.89	.05	357
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	22 145.19	.05	324
		4, 1, 3← 4, 0, 4	Ground			9/2		9/2	22 147.03	.05	324

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}D_2Cl^{35}$	547	5, 1, 4← 5, 0, 5	Ground			7/2		7/2	23 795.5	.05	324
		5, 1, 4← 5, 0, 5	Ground			13/2		13/2	23 796.68	.05	324
		5, 1, 4← 5, 0, 5	Ground						23 798.30	.05	357
		5, 1, 4← 5, 0, 5	Ground			9/2		9/2	23 799.7	.05	324
		5, 1, 4← 5, 0, 5	Ground			11/2		11/2	23 800.9	.05	324
		7, 1, 6← 7, 0, 7	Ground			11/2		11/2	28 448.6	.05	324
		7, 1, 6← 7, 0, 7	Ground			17/2		17/2	28 449.4	.05	324
		7, 1, 6← 7, 0, 7	Ground						28 451.00	.05	357
		7, 1, 6← 7, 0, 7	Ground			13/2		13/2	28 452.5	.05	324
		7, 1, 6← 7, 0, 7	Ground			15/2		15/2	28 453.3	.05	324
$C^bH_3^bC^bH_2^bCl^{35}$	548	Not Reported							20 387.36	.05	324
		Not Reported							20 786.80	.05	324
		Not Reported							20 788.81	.05	324
		Not Reported							20 793.72	.05	324
		Not Reported							20 884.9	.05	324
		Not Reported							20 888.2	.05	324
		Not Reported							22 150.31	.05	324
		Not Reported							22 151.01	.05	324
		Not Reported							24 369.61	.05	324
		Not Reported							26 911.26	.05	324
		Not Reported							26 912.37	.05	324
		Not Reported							26 914.32	.05	324
		Not Reported							26 917.65	.05	324
		Not Reported							26 920.98	.05	324
		Not Reported							26 923.82	.05	324
		Not Reported							26 992.78	.05	324
		Not Reported							26 995.60	.05	324
		Not Reported							27 487.81	.05	324
		Not Reported							27 489.56	.05	324
		Not Reported							27 492.74	.05	324
		Not Reported							27 494.32	.05	324
		Not Reported							29 454.08	.05	324
		Not Reported							29 544.1	.05	324

C_2H_5F $C_s(C_{3v},C_s)$ CH_3CH_2F

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2F^{19}$	C_s	551	36 070.30 M	9 364.54 M	8 199.74 M			−.9164	
$C^{12}H_3C^{12}HDF^{19}$	C_1	552	31 140.2 M	9 252.63 M	7 995.51 M				
g-$C^{12}H_2DC^{12}H_2F^{19}$	C_s	553	32 601.8 M	8 953.99 M	7 866.31 M				
t-$C^{12}H_2DC^{12}H_2F^{19}$	C_s	554	35 693.3 M	8 623.86 M	7 611.59 M				
$C^{12}H_3C^{13}H_2F^{19}$	C_s	555	35 250.1 M	9 365.66 M	8 157.15 M				
$C^{13}H_3C^{12}H_2F^{19}$	C_s	556	35 915.4 M	9 089.05 M	7 980.16 M				
$C^{12}H_2DC^{12}HDF^{19}$ [1]	C_1	557	28 503.6 M	8 825.73 M	7 696.11 M				
$C^{12}HD_2C^{12}HDF^{19}$ [1]	C_1	558	26 206.1 M	8 457.65 M	7 405.06 M				
$C^{12}HDHC^{12}HDF^{19}$ [1]	C_1	559	28 416.3 M	8 872.88 M	7 649.87 M				
$C^{12}DHDC^{12}HDF^{19}$ [1]	C_1	561	28 183.7 M	8 185.21 M	7 187.84 M				
$C^{12}DH_2C^{12}HDF^{19}$ [1]	C_1	562	30 887.7 M	8 528.66 M	7 437.53 M				
$C^{12}D_2HC^{12}HDF^{19}$ [1]	C_1	563	28 101.0 M	8 227.57 M	7 147.50 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
551	1.69 M	1.00 M	0. X		3306		4.359	440 1			

1. Configurations a, b, and c belong to the same isotopic molecular species, as do configurations d, e, and f. Similarly, the gauche and trans- forms belong to the same isotopic molecular species. Since the form is "gauche" as stated in table 1, not "cis" as in table 3, the term "cis" was assumed to be a typographical error. As Bak et al. treated the configurations independently, each configuration is given its own species number.

References:

ABC: 108, 274 D_J: D_{JK}: κ: 108 Δ:

μ: 108 eQq: V: 258 I: 108 ω: 108

Add. Refs.: 236, 323

Torsional frequency = 270 cm^{-1}. Ref: 108.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2F^{19}$	551	1, 0, 1← 0, 0, 0	Ground	A	1					17 530.5		137
		1, 0, 1← 0, 0, 0	Ground							17 549.69		215
		1, 0, 1← 0, 0, 0	Ground							17 564.66		215
		1, 1, 0← 1, 0, 1	Ground	A	1					27 767.7		137
		1, 1, 0← 1, 0, 1	Ground							27 774.33		215
		1, 1, 0← 1, 0, 1	Ground							27 809.78		215
		1, 1, 0← 1, 0, 1	Ground							27 870.71		215
		2, 0, 2← 1, 0, 1	Ground	A	1					35 024.2		137
		2, 0, 2← 1, 0, 1	Ground							35 060.		215
		2, 0, 2← 1, 0, 1	Ground							35 091.16	.10	108
		2, 1, 1← 1, 1, 0	Ground							33 963.77	.10	108
		2, 1, 2← 1, 1, 1	Ground							36 293.37	.10	108
		2, 1, 1← 2, 0, 2	Ground	A	1					28 954.4		137
		2, 1, 1← 2, 0, 2	Ground							28 960.42		215
		2, 1, 1← 2, 0, 2	Ground							28 984.5		215
		2, 1, 1← 2, 0, 2	Ground							29 072.68	.10	108
		2, 2, 1← 3, 1, 2	Ground							25 698.47	.10	108
		3, 0, 3← 2, 1, 2	Ground	E	1					26 935.69		236
		3, 0, 3← 2, 1, 2	Ground	A	1					26 940.54		236
		3, 0, 3← 2, 1, 2	Ground	A	0					26 965.09		236
		3, 1, 3← 2, 2, 0	Ground							32 723.83	.10	108
		3, 1, 2← 3, 0, 3	Ground	A	1					30 802.1		137
		3, 1, 2← 3, 0, 3	Ground							30 808.22		215
		3, 1, 2← 3, 0, 3	Ground							30 945.15		215
		4, 1, 3← 4, 0, 4	Ground							33 568.38	.10	108
		5, 1, 4← 5, 0, 5	Ground							37 042.99	.10	108
		5, 1, 4← 5, 1, 5	Ground	A	1					17 229.8		137
		5, 1, 4← 5, 1, 5	Ground							17 240.53		215
		5, 1, 4← 5, 1, 5	Ground							17 449.71		215
		5, 3, 2← 6, 2, 5	Ground							31 564.84	.10	108
		5, 3, 3← 6, 2, 4	Ground							28 990.30		215
		6, 1, 5← 5, 2, 4	Ground							35 263.45	.10	108
		6, 1, 5← 6, 1, 6	Ground							24 393.70	.10	108
		7, 1, 7← 6, 2, 4	Ground							21 523.36		215
		7, 1, 6← 7, 1, 7	Ground							32 449.89	.10	108
		Not Reported								20 636.57		215
		Not Reported								20 642.17		215
		Not Reported								21 498.03		215
		Not Reported								21 547.94		215
		Not Reported								21 792.83		215
		Not Reported								21 828.32		215
		Not Reported								22 463.5		215
		Not Reported								27 204.33		215
		Not Reported								27 515.68		215
		Not Reported								27 809.78		215
		Not Reported								27 839.05		215
		Not Reported								28 961.55		215
		Not Reported								28 984.5		215
		Not Reported								30 881.71		215
		Not Reported								32 087.89		215

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}HDF^{19}$	552	1, 1, 0← 1, 0, 1	Ground						23 144.5	.1	274
		2, 1, 1← 2, 0, 2	Ground						24 454.2	.1	274
		2, 2, 0← 3, 1, 3	Ground						19 657.6	.1	274
		3, 1, 2← 3, 0, 3	Ground						26 516.7	.1	274
		5, 1, 4← 4, 2, 3	Ground						27 773.2	.1	274
		5, 1, 4← 5, 1, 5	Ground						18 819.1	.1	274
		6, 1, 6← 5, 2, 3	Ground						20 353.4	.1	274
		6, 1, 5← 6, 1, 6	Ground						26 283.3	.1	274
g-$C^{12}H_2DC^{12}H_2F^{19}$	553	1, 1, 0← 1, 0, 1	Ground						24 735.6	.1	274
		2, 1, 1← 2, 0, 2	Ground						25 860.0	.1	274
		2, 2, 0← 3, 1, 3	Ground						25 434.3	.1	274
		2, 2, 1← 3, 1, 2	Ground						18 871.6	.1	274
		3, 0, 3← 2, 1, 2	Ground						27 717.5	.1	274
		3, 1, 2← 3, 0, 3	Ground						27 615.1	.1	274
		5, 1, 4← 4, 2, 3	Ground						19 443.8	.1	274
		5, 3, 2← 6, 2, 5	Ground						20 540.9	.1	274
		6, 1, 5← 6, 1, 6	Ground						22 776.2	.1	274
		7, 1, 7← 6, 2, 4	Ground						26 745.5	.1	274
t-$C^{12}H_2DC^{12}H_2F^{19}$	554	1, 1, 0← 1, 0, 1	Ground						28 081.6	.1	274
		2, 1, 1← 2, 0, 2	Ground						29 122.0	.1	274
		3, 0, 3← 2, 1, 2	Ground						22 509.6	.1	274
		3, 2, 1← 4, 1, 4	Ground						23 056.7	.1	274
		6, 1, 5← 6, 1, 6	Ground						21 217.3	.1	274
		6, 1, 5← 6, 2, 4	Ground						24 955.0	.1	274
		6, 3, 4← 7, 2, 5	Ground						21 542.8	.1	274
$C^{12}H_3C^{13}H_2F^{19}$	555	1, 0, 1← 0, 0, 0	Ground						17 522.7	.1	274
		1, 1, 0← 1, 0, 1	Ground						27 092.7	.1	274
		2, 1, 1← 2, 0, 2	Ground						28 343.1	.1	274
		2, 2, 1← 3, 1, 2	Ground						23 295.7	.1	274
		3, 0, 3← 2, 1, 2	Ground						27 683.8	.1	274
		5, 1, 4← 5, 1, 5	Ground						18 103.9	.1	274
		5, 3, 2← 6, 2, 5	Ground						27 874.3	.1	274
		5, 3, 3← 6, 2, 4	Ground						25 025.1	.1	274
		6, 1, 5← 6, 1, 6	Ground						25 303.5	.1	274
		7, 1, 7← 6, 2, 4	Ground						22 673.8	.1	274
$C^{13}H_3C^{12}H_2F^{19}$	556	1, 1, 0← 1, 0, 1	Ground						27 935.2	.1	274
		2, 2, 1← 3, 1, 2	Ground						27 624.6	.1	274
		3, 0, 3← 2, 1, 2	Ground						25 321.0	.1	274
		3, 2, 1← 4, 1, 4	Ground						19 663.2	.1	274
		6, 1, 5← 6, 1, 6	Ground						23 233.1	.1	274
		6, 3, 3← 6, 2, 6	Ground						18 348.2	.1	274
		7, 1, 7← 6, 2, 4	Ground						18 865.6	.5	274
$C^{12}H_2DC^{12}HDF^{19}$	557	1, 1, 0← 1, 0, 1	Ground						20 806.9	.1	274
		2, 1, 1← 2, 0, 2	Ground						21 984.1	.1	274
		3, 1, 2← 3, 0, 3	Ground						23 837.4	.1	274
		4, 1, 3← 4, 0, 4	Ground						26 466.0	.1	274
		4, 3, 1← 5, 2, 4	Ground						18 868.2	.1	274
		6, 1, 6← 5, 2, 3	Ground						24 395.	1.	274

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2DC^{12}HDF^{19}$	557	6, 1, 5← 6, 1, 6	Ground						23 618.7	.1	274
$C^{12}HD_2C^{12}HDF^{19}$	558	1, 1, 0← 1, 0, 1	Ground						18 800.5	.1	274
		2, 1, 1← 2, 0, 2	Ground						19 898.9	.1	274
		3, 1, 2← 3, 0, 3	Ground						21 630.4	.1	274
		4, 1, 3← 4, 0, 4	Ground						24 090.2	.1	274
		6, 1, 6← 5, 2, 3	Ground						27 245.5	.1	274
		6, 1, 5← 6, 1, 6	Ground						22 001.9	.1	274
$C^{12}HDHC^{12}HDF^{19}$	559	1, 1, 0← 1, 0, 1	Ground						20 766.0	.1	274
		2, 1, 1← 2, 0, 2	Ground						22 045.2	.1	274
		3, 1, 2← 3, 0, 3	Ground						24 066.1	.1	274
		6, 1, 6← 5, 2, 3	Ground						23 322.7	.1	274
		6, 1, 5← 6, 1, 6	Ground						25 551.1	.1	274
$C^{12}DHDC^{12}HDF^{19}$	561	1, 1, 0← 1, 0, 1	Ground						20 995.7	.1	274
		2, 1, 1← 2, 0, 2	Ground						22 029.5	.1	274
		2, 2, 0← 3, 1, 3	Ground						18 418.7	.1	274
		3, 0, 3← 2, 1, 2	Ground						26 935.4	.1	274
		3, 1, 2← 3, 0, 3	Ground						23 647.6	.1	274
		4, 1, 3← 4, 0, 4	Ground						25 928.2	.1	274
		4, 3, 1← 5, 2, 4	Ground						25 823.1	.1	274
		5, 1, 4← 4, 2, 3	Ground						22 613.8	.1	274
		6, 1, 6← 5, 2, 3	Ground						18 610.4	.1	274
		6, 1, 5← 6, 1, 6	Ground						20 875.3	.1	274
$C^{12}DH_2C^{12}HDF^{19}$	562	1, 1, 0← 1, 0, 1	Ground						23 450.0	.1	274
		2, 1, 1← 2, 0, 2	Ground						24 580.2	.1	274
		2, 2, 0← 3, 1, 3	Ground						24 152.3	.1	274
		3, 0, 3← 2, 1, 2	Ground						26 433.5	.1	274
		3, 1, 2← 3, 0, 3	Ground						26 348.0	.1	274
		5, 1, 4← 4, 2, 3	Ground						19 048.2	.1	274
		6, 1, 5← 6, 1, 6	Ground						22 841.0	.1	274
		7, 1, 7← 6, 2, 4	Ground						24 405.0	.1	274
$C^{12}D_2HC^{12}HDF^{19}$	563	1, 1, 0← 1, 0, 1	Ground						20 953.7	.1	274
		2, 1, 1← 2, 0, 2	Ground						22 076.1	.1	274
		2, 2, 0← 3, 1, 3	Ground						18 418.7	.1	274
		3, 0, 3← 2, 1, 2	Ground						27 116.9	.1	274
		3, 1, 2← 3, 0, 3	Ground						23 840.0	.1	274
		4, 1, 3← 4, 0, 4	Ground						26 335.9	.1	274
		4, 3, 1← 5, 2, 4	Ground						25 432.2	.1	274
		5, 1, 4← 4, 2, 3	Ground						23 451.0	.1	274
		6, 1, 6← 5, 2, 3	Ground						17 717.2	.1	274
		6, 1, 5← 6, 1, 6	Ground						22 592.7	.1	274

C_2H_5I $C_s(C_{3v},C_s)$ CH_3CH_2I

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2I^{127}$	C_s	571	29 106.2 M	2 979.2 M	2 797.1 M	.05 [1]	−0.151		

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
571	1.75 M	0.25 M	0. X	−1771	3200						

1. According to a private communication from Kasuya, .05 is the correct value for D_J.

References:

ABC: 283 D_J: 283 D_{JK}: 283 κ: Δ:

μ: 283 eQq: 283 V: 284 I: ω:

Torsional frequency = 230 cm^{-1}. Ref: 284. Centrifugal distortion parameter: $D_K = .36 \pm .05$ MHz. Ref: 283.

Iodoethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2I^{127}$	571	1, 0, 1← 0, 0, 0	Ground			5/2		5/2	5 542.08	.05	283
		1, 0, 1← 0, 0, 0	Ground			7/2		5/2	5 852.44	.05	283
		1, 0, 1← 0, 0, 0	Ground			3/2		5/2	5 988.1	.5	283
		2, 1, 1← 2, 0, 2	Ground			9/2		9/2	26 438.02	.05	283
		2, 1, 1← 2, 0, 2	Ground			7/2		5/2	26 538.5	1.	283
		2, 1, 1← 2, 0, 2	Ground			7/2		7/2	26 620.	2.	283
		2, 1, 1← 2, 0, 2	Ground			5/2		7/2	26 647.50	.05	283
		3, 0, 3← 2, 0, 2	Ground			9/2		9/2	17 070.40	.05	283
		3, 0, 3← 2, 0, 2	Ground			3/2		1/2	17 194.	2.	283
		3, 0, 3← 2, 0, 2	Ground			5/2		3/2	17 212.40	.05	283
		3, 0, 3← 2, 0, 2	Ground			7/2		5/2	17 283.82	.05	283
		3, 0, 3← 2, 0, 2	Ground			11/2		9/2	17 342.28	.05	283
		3, 0, 3← 2, 0, 2	Ground			9/2		7/2	17 354.96	.05	283
		3, 0, 3← 2, 0, 2	Ground			3/2		3/2	17 382.34	.05	283
		3, 1, 2← 2, 1, 1	Ground			7/2		5/2	17 549.70		284
		3, 1, 2← 2, 1, 1	Ground			9/2		7/2	17 574.5		284
		3, 1, 2← 2, 1, 1	Ground			9/2		7/2	17 575.24		284
		3, 1, 2← 2, 1, 1	Ground			11/2		9/2	17 643.66		284
		3, 1, 2← 2, 1, 1	Ground			3/2		3/2	17 662.8		284
		3, 1, 2← 2, 1, 1	Ground			1/2		1/2	17 676.2		284
		3, 1, 3← 2, 1, 2	Ground			5/2		3/2	16 976.8		284
		3, 1, 3← 2, 1, 2	Ground			3/2		1/2	17 007.76		284
		3, 1, 3← 2, 1, 2	Ground			9/2		7/2	17 033.75		284
		3, 1, 3← 2, 1, 2	Ground			9/2		7/2	17 034.84		284
		3, 1, 3← 2, 1, 2	Ground			11/2		9/2	17 096.08		284

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2I^{127}$	571	3, 1, 3← 2, 1, 2	Ground			5/2		5/2	17 110.23		284
		3, 2, 1← 2, 2, 0	Ground			9/2		7/2	17 155.92	.05	283
		3, 2, 1← 2, 2, 0	Ground			7/2		5/2	17 227.84	.05	283
		3, 2, 1← 2, 2, 0	Ground			11/2		9/2	17 443.60	.05	283
		3, 2, 2← 2, 2, 1	Ground			9/2		7/2	17 152.32	.05	283
		3, 2, 2← 2, 2, 1	Ground			7/2		5/2	17 227.84	.05	283
		3, 2, 2← 2, 2, 1	Ground			11/2		9/2	17 438.08	.05	283
		3, 1, 2← 3, 0, 3	Ground			11/2		11/2	26 744.		244
		3, 1, 2← 3, 0, 3	Ground			11/2		11/2	26 745.74	.05	283
		3, 1, 2← 3, 0, 3	Ground			5/2		5/2	26 796.		244
		3, 1, 2← 3, 0, 3	Ground			7/2		7/2	26 835.20	.05	283
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	26 840.46	.05	283
		3, 1, 2← 3, 0, 3	Ground			7/2		9/2	26 843.04	.05	283
		3, 1, 2← 3, 0, 3	Ground			9/2		9/2	26 845.		244
		3, 1, 2← 3, 0, 3	Ground			5/2		7/2	26 900.	1.	283
		3, 1, 2← 3, 0, 3	Ground			3/2		5/2	26 928.	1.	283
		4, 1, 3← 3, 1, 2	Ground			9/2		7/2	23 414.58		284
		4, 1, 3← 3, 1, 2	Ground			11/2		9/2	23 438.13		284
		4, 1, 3← 3, 1, 2	Ground			13/2		11/2	23 467.01		284
		4, 1, 3← 3, 1, 2	Ground			5/2		3/2	23 474.88		284
		4, 1, 4← 3, 1, 3	Ground			7/2		5/2	22 690.03		284
		4, 1, 4← 3, 1, 3	Ground			9/2		7/2	22 709.40		284
		4, 1, 4← 3, 1, 3	Ground			3/2		1/2	22 734.40		284
		4, 1, 4← 3, 1, 3	Ground			11/2		9/2	22 740.73		284
		4, 1, 4← 3, 1, 3	Ground			13/2		11/2	22 759.50		284
		4, 2, 2← 3, 2, 1	Ground			9/2		7/2	23 050.34	.05	283
		4, 2, 2← 3, 2, 1	Ground			11/2		9/2	23 059.77	.05	283
		4, 2, 2← 3, 2, 1	Ground			7/2		5/2	23 090.64	.05	283
		4, 2, 2← 3, 2, 1	Ground			13/2		11/2	23 167.05	.05	283
		4, 2, 3← 3, 2, 2	Ground			9/2		7/2	23 042.24	.05	283
		4, 2, 3← 3, 2, 2	Ground			11/2		9/2	23 050.34	.05	283
		4, 2, 3← 3, 2, 2	Ground			7/2		5/2	23 083.38	.05	283
		4, 2, 3← 3, 2, 2	Ground			13/2		11/2	23 158.50	.05	283
		4, 3, 1← 3, 3, 0	Ground			11/2		9/2	22 968.75	.05	283
		4, 3, 1← 3, 3, 0	Ground			9/2		7/2	22 978.44	.05	283
		4, 3, 1← 3, 3, 0	Ground			7/2		5/2	23 116.56	.05	283
		4, 3, 1← 3, 3, 0	Ground			13/2		11/2	23 214.30	.05	283
		4, 3, 2← 3, 3, 1	Ground			11/2		9/2	22 968.75	.05	283
		4, 3, 2← 3, 3, 1	Ground			9/2		7/2	22 978.44	.05	283
		4, 3, 2← 3, 3, 1	Ground			7/2		5/2	23 116.56	.05	283
		4, 3, 2← 3, 3, 1	Ground			13/2		11/2	23 214.30	.05	283
		4, 1, 3← 4, 0, 4	Ground			3/2		3/2	27 092.56	.05	283
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	27 096.		244
		4, 1, 3← 4, 0, 4	Ground			13/2		13/2	27 110.00	.05	283
		4, 1, 3← 4, 0, 4	Ground			5/2		5/2	27 126.	1.	283
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	27 161.	1.	283
		4, 1, 3← 4, 0, 4	Ground			7/2		7/2	27 166.		244
		4, 1, 3← 4, 0, 4	Ground			9/2		9/2	27 194.28	.05	283
		4, 1, 3← 4, 0, 4	Ground			11/2		11/2	27 196.26	.05	283
		5, 1, 4← 4, 1, 3				9/2		7/2	29 319.70		284

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_i'	F'	F_i	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2I^{127}$	571	5, 1, 4← 4, 1, 3					7/2		5/2	29 320.60		284
		5, 1, 4← 4, 1, 3					11/2		9/2	29 324.64		284
		5, 1, 4← 4, 1, 3					5/2		3/2	29 332.26		284
		5, 1, 4← 4, 1, 3					13/2		11/2	29 337.28		284
		5, 1, 4← 4, 1, 3					15/2		13/2	29 357.16		284
		5, 1, 5← 4, 1, 4	Ground				7/2		5/2	28 389.12		284
		5, 1, 5← 4, 1, 4	Ground				9/2		7/2	28 390.42		284
		5, 1, 5← 4, 1, 4	Ground				11/2		9/2	28 405.78		284
		5, 1, 5← 4, 1, 4					5/2		3/2	28 413.20		284
		5, 1, 5← 4, 1, 4	Ground				13/2		11/2	28 425.40		284
		5, 1, 5← 4, 1, 4	Ground				15/2		13/2	28 433.50		284
		5, 1, 4← 5, 0, 5	Excited	A	0		5/2		5/2	27 430.70		284
		5, 1, 4← 5, 0, 5	Excited	E	0		5/2		5/2	27 432.46		284
		5, 1, 4← 5, 0, 5	Excited	A	0		13/2		13/2	27 501.		284
		5, 1, 4← 5, 0, 5	Excited	E	0		13/2		13/2	27 502.		284
		5, 1, 4← 5, 0, 5	Excited	A	0		11/2		11/2	27 528.10		284
		5, 1, 4← 5, 0, 5	Excited	E	0		11/2		11/2	27 529.56		284
		5, 1, 4← 5, 0, 5	Ground				5/2		5/2	27 562.46		284
		5, 1, 4← 5, 0, 5	Ground				5/2		5/2	27 565.		244
		5, 1, 4← 5, 0, 5	Ground				9/2		9/2	27 593.5		284
		5, 1, 4← 5, 0, 5	Ground				15/2		15/2	27 595.		244
		5, 1, 4← 5, 0, 5	Ground				7/2		7/2	27 596.		284
		5, 1, 4← 5, 0, 5	Ground				7/2		7/2	27 596.0	1.	283
		5, 1, 4← 5, 0, 5	Ground				15/2		15/2	27 597.48	.05	283
		5, 1, 4← 5, 0, 5	Ground				15/2		15/2	27 597.48		284
		5, 1, 4← 5, 0, 5	Ground				13/2		13/2	27 638.		244
		5, 1, 4← 5, 0, 5	Ground				13/2		13/2	27 639.18	.05	283
		5, 1, 4← 5, 0, 5	Ground				13/2		13/2	27 639.18		284
		5, 1, 4← 5, 0, 5	Ground				11/2		11/2	27 663.		244
		5, 1, 4← 5, 0, 5	Ground				11/2		11/2	27 664.54	.05	283
		5, 1, 4← 5, 0, 5	Ground				11/2		11/2	27 664.54		284
		6, 1, 5← 6, 0, 6	Excited				7/2		7/2	28 154.7	.5	284
		6, 1, 5← 6, 0, 6	Excited	A	0		9/2		9/2	28 171.66		284
		6, 1, 5← 6, 0, 6	Excited	E	0		9/2		9/2	28 173.18		284
		6, 1, 5← 6, 0, 6	Excited	A	0		17/2		17/2	28 186.94		284
		6, 1, 5← 6, 0, 6	Excited	E	0		17/2		17/2	28 188.82		284
		6, 1, 5← 6, 0, 6	Excited	A	0		11/2		11/2	28 219.44		284
		6, 1, 5← 6, 0, 6	Excited	E	0		11/2		11/2	28 221.33		284
		6, 1, 5← 6, 0, 6	Excited	A	0		15/2		15/2	28 235.42		284
		6, 1, 5← 6, 0, 6	Excited	E	0		15/2		15/2	28 237.20		284
		6, 1, 5← 6, 0, 6	Excited				13/2		13/2	28 246.1	.5	284
		6, 1, 5← 6, 0, 6	Ground				7/2		7/2	28 264.34		284
		6, 1, 5← 6, 0, 6	Ground				9/2		9/2	28 275.88		284
		6, 1, 5← 6, 0, 6	Ground				17/2		17/2	28 291.66		284
		6, 1, 5← 6, 0, 6	Ground				11/2		11/2	28 324.08		284
		6, 1, 5← 6, 0, 6	Ground				15/2		15/2	28 339.12		284
		6, 1, 5← 6, 0, 6	Ground				13/2		13/2	28 347.34		284

C_2H_6O $C_s(C_{3v},C_s,C_s)$ CH_3CH_2OH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2O^{16}H$	C_s	581	33 326.64 M	9 112.96 M	8 019.39 M			−.9136	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
581	1.18 M	1.46 M	0. X		3000						

References:

ABC: 268 D_J: D_{JK}: κ: 268 Δ:
μ: 268 eQq: V: 113 I: ω:
Add. Ref.: 369

Ethanol

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2O^{16}H$	581	1, 0, 1← 0, 0, 0	Ground						17 132.35		268
		1, 1, 0← 1, 0, 1	Ground						25 307.25	.01	268
		2, 1, 1← 2, 0, 2	Ground						26 437.15	.01	268
		3, 1, 2← 2, 2, 1	Ground						19 629.0	.1	268
		4, 2, 3← 5, 1, 4	Ground						19 343.9	.1	268
		5, 1, 4← 5, 1, 5	Ground						16 399.85	.01	268
		6, 2, 4← 5, 3, 3	Ground						19 006.19	.01	268
		6, 2, 5← 5, 3, 2	Ground						21 501.		268
		6, 1, 5← 6, 1, 6	Ground						22 890.95	.01	268
		7, 3, 5← 8, 2, 6	Ground						18 772.5	.1	268
		9, 1, 8← 8, 3, 5	Ground						23 769.		268
		9, 3, 7← 8, 4, 4	Ground						18 367.8	.1	268
		10, 3, 7←11, 1,10	Ground						20 513.18	.01	268
		10, 4, 6←11, 3, 9	Ground						20 285.		268
		10, 4, 7←11, 3, 8	Ground						22 474.13	.01	268
		Not Reported							21 572.00	.01	268 [1]
		Not Reported							22 820.		19
		Not Reported							23 081.		19
		Not Reported							23 148.		19
		Not Reported							23 428.83	.01	268 [1]
		Not Reported							23 555.		19
		Not Reported							23 605.		19
		Not Reported							24 288.71	.01	268 [1]
		Not Reported							24 295.		19
		Not Reported							24 369.		19
		Not Reported							24 383.24	.01	268 [1]
		Not Reported							24 384.04	.01	268 [1]
		Not Reported							24 385.		19
		Not Reported							25 069.		19
		Not Reported							25 307.03	.01	268
		Not Reported							26 148.24	.01	268 [1]
		Not Reported							26 436.88	.01	268

1. For the following lines, quoted from Schafer's thesis, limiting J quantum numbers are given as follows:
24,288.71 MHz. $J \geq 3$ 26,148.24 MHz. $J \geq 7$
21,572.00 MHz. $J \geq 4$ 24,383.24 MHz. $J \geq 8$
23,428.83 MHz. $J \geq 4$ 24,384.04 MHz. $J \geq 8$

In all cases, $\Delta J = 0$.

C_2H_6O $C_{2v}(C_s,C_{2v},C_s)$ $(CH_3)_2O$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_2O^{16}$	C_{2v}	591	38 788.5 M	10 056.6 M	8 886.9 M				
$(C^{12}D_3)_2O^{16}$	C_{2v}	592	25 696.4 M	7 483.9 M	6 798.1 M				
$(C^{12}D_3)(C^{12}H_3)O^{16}$	C_s	593	30 912.7 M	8 635.5 M	7 747.7 M				
$(C^{13}H_3)(C^{12}H_3)O^{16}$	C_s	594	38 615.6 M	9 795.6 M	8 673.5 M				
$(C^{12}H_3)_2O^{18}$	C_{2v}	595	37 172.1 M	10 058.2 M	8 799.4 M				
s-$(C^{12}H_2D)(C^{12}H_3)O^{16}$	C_s	596	38 281.6 M	9 309.1 M	8 277.9 M				
a-$(C^{12}H_2D)(C^{12}H_3)O^{16}$	C_1	597	34 764.1 M	9 642.3 M	8 537.2 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
591	0. X	1.302 M	0. X		2720						
592	0. X	1.319 M	0. X								

References:

ABC: 360 D_J: D_{JK}: κ: Δ:

μ: 360 eQq: V: 243 I: ω:

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2O^{16}$	591	1, 1, 1← 0, 0, 0	Ground						47 675.4	.2	360
		1, 1, 0← 1, 0, 1	Excited						29 850.	20.	342
		1, 1, 0← 1, 0, 1	Excited						29 880.	20.	342
		1, 1, 0← 1, 0, 1	Ground						29 901.4	.2	360
		1, 1, 0← 1, 0, 1	Excited						29 931.	5.	342
		1, 1, 0← 1, 0, 1	Excited						29 937.	5.	342
		1, 1, 0← 1, 0, 1	Excited						29 946.2	.2	342
		1, 1, 0← 1, 0, 1	Excited						29 957.6	1.	342
		1, 1, 0← 1, 0, 1	Excited						29 971.1	1.	342
		1, 1, 0← 1, 0, 1	Excited						29 976.5	1.	342
		1, 1, 0← 1, 0, 1	Excited						29 990.8	1.	342
		2, 0, 2← 1, 1, 1	Ground						9 119.7	.5	360
		2, 1, 1← 2, 0, 2	Excited						31 055.	5.	342
		2, 1, 1← 2, 0, 2	Excited						31 065.	5.	342
		2, 1, 1← 2, 0, 2	Excited						31 085.	5.	342
		2, 1, 1← 2, 0, 2	Excited						31 090.	5.	342
		2, 1, 1← 2, 0, 2	Excited						31 095.0	.2	342
		2, 1, 1← 2, 0, 2	Excited						31 103.	1.	342
		2, 1, 1← 2, 0, 2	Ground						31 106.3	.2	360
		2, 1, 1← 2, 0, 2	Excited						31 125.	20.	342
		2, 1, 1← 2, 0, 2	Excited						31 135.	20.	342
		2, 1, 1← 2, 0, 2	Excited						31 145.	20.	342
		2, 1, 1← 2, 0, 2	Excited						31 180.	20.	342
		3, 0, 3← 2, 1, 2	Ground						29 092.1	.5	360
		3, 1, 2← 2, 2, 1	Ground						27 629.5	.5	360
		3, 1, 3← 2, 2, 0	Ground						34 682.5	.5	360
		3, 1, 2← 3, 0, 3	Excited						32 748.4	.2	342
		3, 1, 2← 3, 0, 3	Excited						32 872.9	.2	342
		3, 1, 2← 3, 0, 3	Excited						32 897.0	1.	342
		3, 1, 2← 3, 0, 3	Excited						32 898.5	1.	342
		3, 1, 2← 3, 0, 3	Excited						32 945.	20.	342
		3, 1, 2← 3, 0, 3	Excited						32 965.	20.	342
		3, 1, 2← 3, 0, 3	Excited						32 970.	20.	342
		3, 1, 2← 3, 0, 3	Ground						32 978.5	.5	360
		3, 1, 2← 3, 0, 3	Excited						33 020.	20.	342
		3, 1, 2← 3, 0, 3	Excited						33 030.	20.	342
		3, 1, 2← 3, 0, 3	Excited						33 060.	20.	342
		4, 1, 3← 4, 0, 4	Excited						35 325.	20.	342
		4, 1, 3← 4, 0, 4	Excited						35 335.	20.	342
		4, 1, 3← 4, 0, 4	Excited						35 390.	20.	342
		4, 1, 3← 4, 0, 4	Excited						35 525.	20.	342
		4, 1, 3← 4, 0, 4	Excited						35 550.	20.	342
		4, 1, 3← 4, 0, 4	Excited						35 575.	20.	342
		4, 1, 3← 4, 0, 4	Ground						35 593.4	.5	360
		4, 1, 3← 4, 0, 4	Excited						35 615.	20.	342
		4, 1, 3← 4, 0, 4	Excited						35 660.	20.	342
		4, 1, 3← 4, 0, 4	Ground						35 670.	20.	342
		5, 1, 4← 5, 0, 5	Ground						39 047.1	.5	360
		6, 1, 5← 6, 0, 5	Ground						43 450.	20.	342
		9, 2, 7← 8, 3, 6	Ground						31 980.	20.	342

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2O^{16}$	591	12, 3, 9←11, 4, 8	Ground						26 598.6	.2	342
		Not Reported	Ground						8 060.	1.	342
		Not Reported	Ground						8 074.	1.	342
		Not Reported	Ground						8 114.	1.	342
		Not Reported	Ground						8 165.	5.	342
		Not Reported	Ground						8 898.	5.	342
		Not Reported	Ground						8 911.	5.	342
		Not Reported	Ground						8 955.	5.	342
		Not Reported	Ground						9 150.	5.	342
		Not Reported	Ground						23 275.	20.	342
		Not Reported	Ground						24 310.	20.	342
		Not Reported	Ground						24 425.	20.	342
		Not Reported	Ground						28 200.	20.	342
		Not Reported	Ground						29 430.	20.	342
		Not Reported	Ground						30 350.	20.	342
		Not Reported	Ground						32 425.	20.	342
		Not Reported	Ground						35 030.	20.	342
		Not Reported	Ground						35 140.	20.	342
		Not Reported	Ground						36 440.	20.	342
		Not Reported	Ground						36 450.	20.	342
		Not Reported	Ground						36 870.	20.	342
		Not Reported	Ground						37 890.	20.	342
		Not Reported	Ground						38 660.	20.	342
		Not Reported	Ground						38 675.	20.	342
		Not Reported	Ground						38 690.	20.	342
		Not Reported	Ground						39 800.	20.	342
$(C^{12}D_3)_2O^{16}$	592	1, 1, 1← 0, 0, 0	Ground						32 494.5	.2	360
		1, 1, 0← 1, 0, 1	Ground						18 898.3	.2	360
		1, 1, 0← 1, 0, 1	Ground						18 912.8	.2	342
		2, 0, 2← 1, 1, 1	Ground						10 332.3	.5	360
		2, 1, 1← 2, 0, 2	Ground						19 603.2	.2	360
		3, 0, 3← 2, 1, 2	Ground						25 223.6	.5	360
		3, 1, 2← 3, 0, 3	Ground						20 695.5	.5	360
		4, 1, 3← 4, 0, 4	Excited						22 072.2	.2	342
		4, 1, 3← 4, 0, 4	Excited						22 081.4	.2	342
		4, 1, 3← 4, 0, 4	Excited						22 208.3	.2	342
		4, 1, 3← 4, 0, 4	Excited						22 213.6	.2	342
		4, 1, 3← 4, 0, 4	Ground						22 216.9	.5	360
		5, 1, 4← 5, 0, 5	Ground						24 219.8	.5	360
		Not Reported	Ground						10 400.	5.	342
		Not Reported	Ground						10 415.	5.	342
		Not Reported	Ground						10 425.	5.	342
		Not Reported	Ground						19 140.	20.	342
		Not Reported	Ground						19 607.1	.2	342
		Not Reported	Ground						19 650.	20.	342
		Not Reported	Ground						19 720.	20.	342
		Not Reported	Ground						22 045.	2.	342
		Not Reported	Ground						22 065.	2.	342
		Not Reported	Ground						24 170.	20.	342

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}D_3)_2O^{16}$	592	Not Reported	Ground						24 180.	20.	342
		Not Reported	Ground						24 185.	20.	342
		Not Reported	Ground						32 185.4	.2	342
		Not Reported	Ground						40 185.4	20.	342
$(C^{12}D_3)(C^{12}H_3)O^{16}$	593	1, 1, 1← 0, 0, 0	Ground						38 659.	1.0	342
		1, 1, 0← 1, 0, 1	Ground						23 164.9	.2	360
		1, 1, 0← 1, 0, 1	Excited						23 175.	20.	342
		2, 0, 2← 1, 1, 1	Ground						10 463.1	.2	360
		2, 1, 1← 2, 0, 2	Ground						24 078.7	.2	360
		3, 0, 3← 2, 1, 2	Ground						27 630.0	.1	360
		4, 1, 3← 4, 0, 4	Ground						27 478.5	.5	360
		Not Reported	Ground						24 035.	20.	342
		Not Reported	Ground						24 055.	20.	342
		Not Reported	Ground						24 075.	20.	342
		Not Reported	Ground						24 115.	20.	342
		Not Reported	Ground						24 125.	20.	342
		Not Reported	Ground						38 638.	.5	342
		Not Reported	Ground						38 649.5	.5	342
$(C^{13}H_3)(C^{12}H_3)O^{16}$	594	1, 1, 0← 1, 0, 1	Ground						29 942.1	.2	360
		2, 0, 2← 1, 1, 1	Ground						8 086.2	.2	360
		2, 1, 1← 2, 0, 2	Ground						31 096.3	.2	360
		3, 0, 3← 2, 1, 2	Ground						27 548.3	.5	360
		3, 1, 2← 3, 0, 3	Ground						32 887.4	.5	360
$(C^{12}H_3)_2O^{18}$	595	1, 1, 0← 1, 0, 1	Ground						28 372.7	.2	360
		1, 1, 0← 1, 0, 1	Excited						29 635.	20.	342
		1, 1, 0← 1, 0, 1	Excited						29 660.	20.	342
		1, 1, 0← 1, 0, 1	Excited						29 695.	20.	342
		1, 1, 0← 1, 0, 1	Excited						29 710.	20.	342
		1, 1, 0← 1, 0, 1	Excited						29 720.	20.	342
		2, 0, 2← 1, 1, 1	Ground						10 558.5	.2	360
		2, 1, 1← 2, 0, 2	Ground						29 674.3	.2	360
		3, 0, 3← 2, 1, 2	Ground						30 503.0	.5	360
		3, 1, 2← 3, 0, 3	Ground						31 706.2	.5	360
s-$(C^{12}H_2D)(C^{12}H_3)O^{16}$	596	1, 1, 0← 1, 0, 1	Ground						30 003.6	.2	360
		2, 1, 1← 2, 0, 2	Ground						31 061.8	.2	360
		3, 0, 3← 2, 1, 2	Ground						24 684.6	.2	360
		3, 1, 2← 3, 0, 3	Ground						32 699.5	.5	360
		5, 1, 5← 4, 2, 2	Ground						8 828.6	.5	360
		Not Reported	Ground						8 890.	5.	342
		Not Reported	Ground						8 950.	5.	342
		Not Reported	Ground						8 960.	5.	342
		Not Reported	Ground						24 640.	20.	342
		Not Reported	Ground						24 660.	20.	342
		Not Reported	Ground						24 700.	20.	342
		Not Reported	Ground						24 750.	20.	342
		Not Reported	Ground						24 785.	20.	342
		Not Reported	Ground						24 875.	20.	342
		Not Reported	Ground						24 900.	20.	342
		Not Reported	Ground						24 980.	20.	342

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
s-($C^{12}H_2D$)($C^{12}H_3$)O^{16}	596	Not Reported	Ground						24 995.	20.	342
		Not Reported	Ground						25 000.	20.	342
		Not Reported	Ground						25 020.	20.	342
		Not Reported	Ground						25 030.	20.	342
		Not Reported	Ground						25 035.	20.	342
		Not Reported	Ground						27 200.	20.	342
		Not Reported	Ground						27 240.	20.	342
		Not Reported	Ground						27 250.	20.	342
		Not Reported	Ground						27 290.	20.	342
		Not Reported	Ground						27 325.	20.	342
		Not Reported	Ground						29 135.	20.	342
		Not Reported	Ground						29 140.	20.	342
		Not Reported	Ground						29 150.	20.	342
		Not Reported	Ground						29 520.	20.	342
		Not Reported	Ground						29 535.	20.	342
		Not Reported	Ground						29 540.	20.	342
		Not Reported	Ground						29 550.	20.	342
		Not Reported	Ground						29 555.	20.	342
		Not Reported	Ground						29 560.	20.	342
		Not Reported	Ground						29 590.	20.	342
		Not Reported	Ground						29 600.	20.	342
		Not Reported	Ground						29 630.	20.	342
		Not Reported	Ground						29 680.	20.	342
		Not Reported	Ground						29 730.	20.	342
		Not Reported	Ground						29 835.	20.	342
		Not Reported	Ground						29 880.	20.	342
		Not Reported	Ground						29 895.	20.	342
		Not Reported	Ground						31 000.	20.	342
		Not Reported	Ground						31 200.	20.	342
a-($C^{12}H_2D$)($C^{12}H_3$)O^{16}	597	1, 1, 0← 1, 0, 1	Ground						26 226.9	.2	360
		2, 0, 2← 1, 1, 1	Ground						11 201.6	.2	360
		2, 1, 1← 2, 0, 2	Ground						27 367.7	.2	360
		3, 0, 3← 2, 1, 2	Ground						30 343.3	.5	360
		3, 1, 2← 3, 0, 3	Ground						29 145.4	.5	360

C_2H_6S $C_{2v}(C_{3v},C_{3v},C_{2v})$ $(CH_3)_2S$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_2S^{32}$	C_{2v}	601	17 809.82 M	7 621.03 M	5 717.79 M				6.3049
$(C^{12}H_3)_2S^{34}$	C_{2v}	602	17 398.72 M	7 621.36 M	5 674.63 M				6.3002
$C^{13}H_3S^{32}C^{12}H_3$	C_s	603	17 612.44 M	7 412.37 M	5 579.66 M				6.3016
s-$C^{12}H_2DS^{32}C^{12}H_3$	C_s	604	17 794.97 M	7 069.04 M	5 401.69 M				6.3344
a-$C^{12}H_2DS^{32}C^{12}H_3$	C_1	605	16 557.01 M	7 335.25 M	5 512.05 M				7.6369
$C^{12}H_3S^{32}C^{12}D_3$	C_s	606	15 480.51 M	6 595.97 M	5 067.40 M				9.5369

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
601	0. X	1.50 M	0. X		2132	6					
606					2118	3					

References:

ABC: 332 D_J: D_{JK}: κ: Δ: 332

μ: 332 eQq: V: 332 I: ω:

Add. Refs: 279, 311, 334

For species 601, the coupling parameter is: $I_\alpha = 3.204$ amu Å^2.
For species 606, the coupling parameters are: $I_{\alpha_1} = 3.204$ amu Å^2, and $I_\alpha = 6.403$ amu Å^2. Its rotational constants for first excited torsional states are: for CD_3, A = 15486.59 MHz, B = 6570.58 MHz, and C = 5060.61 MHz; for CH_3, A = 15409.49 MHz, B = 6564.46 MHz, and C = 5057.68 MHz. Ref: 332.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2S^{32}$	601	1, 1, 1← 0, 0, 0	Ground							23 527.26	.05	356
		1, 1, 1← 0, 0, 0	Ground							23 527.50	.05	356
		1, 1, 1← 0, 0, 0	Ground	AA	0					23 527.60	.05	332
		1, 1, 1← 0, 0, 0	Ground							23 527.73	.05	356
		1, 1, 0← 1, 0, 1	Ground							12 091.72	.05	356
		1, 1, 0← 1, 0, 1	Ground							12 091.96	.05	356
		1, 1, 0← 1, 0, 1	Ground	AA	0					12 092.03	.05	332
		1, 1, 0← 1, 0, 1	Ground							12 092.20	.05	356
		2, 0, 2← 1, 1, 1	Ground							16 246.12	.05	356
		2, 0, 2← 1, 1, 1	Ground	AA	0					16 246.27	.05	332
		2, 0, 2← 1, 1, 1	Ground							16 246.28	.05	356
		2, 0, 2← 1, 1, 1	Ground							16 246.45	.05	356
		2, 1, 2← 1, 0, 1	Ground							34 962.82	.05	356
		2, 1, 2← 1, 0, 1	Ground							34 963.06	.05	356
		2, 1, 2← 1, 0, 1	Ground							34 963.29	.05	356
		2, 2, 1← 1, 1, 0	Ground							59 144.77	.05	356
		2, 2, 1← 1, 1, 0	Ground							59 144.89	.05	356
		2, 2, 1← 1, 1, 0	Ground							59 145.58	.05	356
		2, 2, 1← 1, 1, 0	Ground							59 146.32	.05	356
		2, 1, 1← 2, 0, 2	Ground							14 237.62	.05	356
		2, 1, 1← 2, 0, 2	Ground	AA	0					14 237.82	.05	332
		2, 1, 1← 2, 0, 2	Ground							14 237.88	.05	356
		2, 1, 1← 2, 0, 2	Ground							14 238.16	.05	356
		2, 1, 2← 2, 2, 1	Ground							12 142.83	.05	356
		2, 1, 2← 2, 2, 1	Ground							12 143.37	.05	356
		2, 1, 2← 2, 2, 1	Ground							12 143.86	.05	356
		2, 1, 2← 2, 2, 1	Ground							12 143.99	.05	356
		2, 2, 0← 2, 1, 1	Ground							30 806.69	.05	356
		2, 2, 0← 2, 1, 1	Ground							30 806.83	.05	356
		2, 2, 0← 2, 1, 1	Ground							30 807.35	.05	356
		2, 2, 0← 2, 1, 1	Ground							30 807.95	.05	356
		2, 2, 1← 2, 1, 2	Ground							36 273.68	.05	356
		2, 2, 1← 2, 1, 2	Ground							36 273.81	.05	356
		2, 2, 1← 2, 1, 2	Ground							36 274.50	.05	356
		2, 2, 1← 2, 1, 2	Ground							36 275.25	.05	356
		3, 0, 3← 2, 1, 2	Ground							30 542.49	.05	356
		3, 0, 3← 2, 1, 2	Ground							30 542.60	.05	356
		3, 0, 3← 2, 1, 2	Ground							30 542.70	.05	356
		3, 1, 2← 3, 0, 3	Ground							17 874.98	.05	356
		3, 1, 2← 3, 0, 3	Ground	EE	0					17 875.28	.05	332
		3, 1, 2← 3, 0, 3	Ground							17 875.29	.05	356
		3, 1, 2← 3, 0, 3	Ground	AA	0					17 875.58	.05	332
		3, 1, 2← 3, 0, 3	Ground							17 875.61	.05	356
		3, 2, 1← 3, 1, 2	Ground							29 060.28	.05	356
		3, 2, 1← 3, 1, 2	Ground							29 060.86	.05	356
		3, 2, 1← 3, 1, 2	Ground							29 061.45	.05	356
		3, 2, 2← 3, 1, 3	Ground							39 272.12	.05	356
		3, 2, 2← 3, 1, 3	Ground							39 272.87	.05	356
		3, 2, 2← 3, 1, 3	Ground							39 273.64	.05	356
		4, 1, 3← 3, 2, 2	Ground							28 738.25	.05	356

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2S^{32}$	601	4, 1, 3← 3, 2, 2	Ground							28 738.69	.05	356
		4, 1, 3← 3, 2, 2	Ground							28 739.14	.05	356
		4, 1, 3← 4, 0, 4	Ground							23 353.25	.05	356
		4, 1, 3← 4, 0, 4	Ground							23 353.31	.05	332
		4, 1, 3← 4, 0, 4	Ground							23 353.64	.05	356
		4, 1, 3← 4, 0, 4	Ground	EE	0					23 353.66	.05	332
		4, 1, 3← 4, 0, 4	Ground	AA	0					23 354.03	.05	332
		4, 1, 3← 4, 0, 4	Ground							23 354.03	.05	356
		4, 2, 2← 4, 1, 3	Ground							27 832.08	.05	356
		4, 2, 2← 4, 1, 3	Ground							27 832.63	.05	356
		4, 2, 2← 4, 1, 3	Ground							27 833.20	.05	356
		4, 2, 3← 4, 1, 4	Ground							43 321.37	.05	356
		4, 2, 3← 4, 1, 4	Ground							43 322.18	.05	356
		4, 2, 3← 4, 1, 4	Ground							43 322.98	.05	356
		4, 3, 1← 4, 2, 2	Ground							53 188.71	.05	356
		4, 3, 1← 4, 2, 2	Ground							53 189.22	.05	356
		4, 3, 1← 4, 2, 2	Ground							53 189.91	.05	356
		4, 3, 1← 4, 2, 2	Ground							53 190.85	.05	356
		4, 3, 2← 4, 2, 3	Ground							56 459.09	.05	356
		4, 3, 2← 4, 2, 3	Ground							56 459.59	.05	356
		4, 3, 2← 4, 2, 3	Ground							56 460.57	.05	356
		4, 3, 2← 4, 2, 3	Ground							56 461.78	.05	356
		5, 2, 3← 4, 3, 2	Ground	AA	0					17 073.67	.05	332
		5, 2, 3← 4, 3, 2	Ground	EE	0					17 074.70	.05	332
		5, 2, 3← 4, 3, 2	Ground	AE	0					17 075.45	.05	332
		5, 2, 3← 4, 3, 2	Ground	EA	0					17 075.97	.05	332
		5, 1, 4← 5, 0, 5	Ground							30 822.84	.05	356
		5, 1, 4← 5, 0, 5	Ground							30 823.32	.05	356
		5, 1, 4← 5, 0, 5	Ground							30 823.80	.05	356
		5, 2, 3← 5, 1, 4	Ground							27 787.09	.05	356
		5, 2, 3← 5, 1, 4	Ground							27 787.63	.05	356
		5, 2, 3← 5, 1, 4	Ground							27 788.17	.05	356
		5, 2, 4← 5, 1, 5	Ground							48 418.84	.05	356
		5, 2, 4← 5, 1, 5	Ground							48 419.72	.05	356
		5, 2, 4← 5, 1, 5	Ground							48 420.60	.05	356
		5, 3, 2← 5, 2, 3	Ground							50 797.50	.05	356
		5, 3, 2← 5, 2, 3	Ground							50 798.49	.05	356
		5, 3, 2← 5, 2, 3	Ground							50 799.48	.05	356
		6, 1, 6← 5, 2, 3	Ground							17 047.35	.05	356
		6, 1, 6← 5, 2, 3	Ground	AA	0					17 047.37	.05	332
		6, 1, 6← 5, 2, 3	Ground							17 048.23	.05	356
		6, 1, 6← 5, 2, 3	Ground	EE	0					17 048.25	.05	332
		6, 1, 6← 5, 2, 3	Ground							17 049.12	.05	356
		6, 2, 4← 5, 3, 3	Ground							34 652.35	.05	356
		6, 2, 4← 5, 3, 3	Ground							34 653.19	.05	356
		6, 2, 4← 5, 3, 3	Ground							34 653.95	.05	356
		6, 2, 4← 5, 3, 3	Ground							34 654.08	.05	356
		6, 2, 5← 5, 3, 2	Ground	AA	0					20 768.25	.05	332
		6, 2, 5← 5, 3, 2	Ground							20 768.31	.05	356
		6, 2, 5← 5, 3, 2	Ground	EE	0					20 769.17	.05	332

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2S^{32}$	601	6, 2, 5← 5, 3, 2	Ground							20 769.23	.05	356
		6, 2, 5← 5, 3, 2	Ground							20 770.09	.05	332
		6, 2, 5← 5, 3, 2	Ground							20 770.10	.05	356
		6, 2, 5← 5, 3, 2	Ground							20 770.21	.05	356
		6, 1, 5← 6, 0, 6	Ground							40 068.47	.05	356
		6, 1, 5← 6, 0, 6	Ground							40 069.09	.05	356
		6, 1, 5← 6, 0, 6	Ground							40 069.70	.05	356
		6, 2, 4← 6, 1, 5	Ground							29 452.88	.05	356
		6, 2, 4← 6, 1, 5	Ground							29 453.41	.05	356
		6, 2, 4← 6, 1, 5	Ground							29 453.93	.05	356
		6, 2, 5← 6, 1, 6	Ground							54 518.60	.05	356
		6, 2, 5← 6, 1, 6	Ground							54 519.54	.05	356
		6, 2, 5← 6, 1, 6	Ground							54 520.48	.05	356
		6, 3, 3← 6, 2, 4	Ground							47 775.11	.05	356
		6, 3, 3← 6, 2, 4	Ground							47 776.06	.05	356
		6, 3, 3← 6, 2, 4	Ground							47 777.01	.05	356
		6, 3, 4← 6, 2, 5	Ground							59 588.00	.05	356
		6, 3, 4← 6, 2, 5	Ground							59 589.10	.05	356
		6, 3, 4← 6, 2, 5	Ground							59 590.19	.05	356
		6, 4, 3← 7, 3, 4	Ground	AA	0					20 590.99	.05	332
		6, 4, 3← 7, 3, 4	Ground	EE	0					20 592.70	.05	332
		6, 4, 3← 7, 3, 4	Ground	AE	0					20 593.52	.05	332
		6, 4, 3← 7, 3, 4	Ground	EA	0					20 595.36	.05	332
		7, 1, 7← 6, 2, 4	Ground							16 647.89	.05	356
		7, 1, 7← 6, 2, 4	Ground							16 648.91	.05	356
		7, 1, 7← 6, 2, 4	Ground							16 649.94	.05	356
		7, 2, 6← 6, 3, 3	Ground							30 398.95	.05	356
		7, 2, 6← 6, 3, 3	Ground							30 399.88	.05	356
		7, 2, 6← 6, 3, 3	Ground							30 400.80	.05	356
		7, 3, 5← 6, 4, 2	Ground	EE	0					16 892.80	.05	332
		7, 3, 5← 6, 4, 2	Ground							16 894.33	.05	332
		7, 3, 5← 6, 4, 2	Ground	AA	0					76 891.91	.05	332
		7, 1, 6← 7, 0, 7	Ground							50 547.58	.05	356
		7, 1, 6← 7, 0, 7	Ground							50 548.33	.05	356
		7, 1, 6← 7, 0, 7	Ground							50 549.11	.05	356
		7, 2, 5← 7, 1, 6	Ground							33 210.66	.05	356
		7, 2, 5← 7, 1, 6	Ground							33 211.20	.05	356
		7, 2, 5← 7, 1, 6	Ground							33 211.73	.05	356
		7, 2, 6← 7, 1, 7	Ground							61 526.00	.05	356
		7, 2, 6← 7, 1, 7	Ground							61 527.05	.05	356
		7, 2, 6← 7, 1, 7	Ground							61 528.10	.05	356
		7, 3, 4← 7, 2, 5	Ground							44 762.10	.05	356
		7, 3, 4← 7, 2, 5	Ground							44 762.99	.05	356
		7, 3, 4← 7, 2, 5	Ground							44 763.86	.05	356
		7, 3, 5← 7, 2, 6	Ground							62 433.00	.05	356
		7, 3, 5← 7, 2, 6	Ground							62 434.12	.05	356
		7, 3, 5← 7, 2, 6	Ground							62 435.22	.05	356
		8, 2, 7← 7, 3, 4	Ground							37 805.82	.05	356
		8, 2, 7← 7, 3, 4	Ground							37 807.71	.05	356
		8, 2, 7← 7, 3, 4	Ground							37 846.77	.05	356

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2S^{32}$	601	8, 1, 7← 8, 0, 8	Ground							61 594.68	.05	356
		8, 1, 7← 8, 0, 8	Ground							61 595.62	.05	356
		8, 1, 7← 8, 0, 8	Ground							61 596.57	.05	356
		8, 2, 6← 8, 1, 7	Ground							39 285.65	.05	356
		8, 2, 6← 8, 1, 7	Ground							39 286.23	.05	356
		8, 2, 6← 8, 1, 7	Ground							39 286.80	.05	356
		8, 3, 5← 8, 2, 6	Ground							42 572.36	.05	356
		8, 3, 5← 8, 2, 6	Ground							42 573.17	.05	356
		8, 3, 5← 8, 2, 6	Ground							42 573.97	.05	356
		9, 2, 8← 8, 3, 5	Ground							42 361.59	.05	356
		9, 2, 8← 8, 3, 5	Ground							42 362.56	.05	356
		9, 2, 8← 8, 3, 5	Ground							42 363.55	.05	356
		9, 2, 7← 9, 1, 8	Ground							47 641.04	.05	356
		9, 2, 7← 9, 1, 8	Ground							47 641.70	.05	356
		9, 2, 7← 9, 1, 8	Ground							47 642.37	.05	356
		9, 3, 6← 9, 2, 7	Ground							41 972.48	.05	356
		9, 3, 6← 9, 2, 7	Ground							41 973.22	.05	356
		9, 3, 6← 9, 2, 7	Ground							41 973.95	.05	356
		10, 2, 9← 9, 3, 6	Ground							43 636.47	.05	356
		10, 2, 9← 9, 3, 6	Ground							43 637.52	.05	356
		10, 2, 9← 9, 3, 6	Ground							43 638.57	.05	356
		10, 5, 5← 9, 6, 4	Ground	AA	0					14 515.57	.05	332
		10, 5, 5← 9, 6, 4	Ground	EE	0					14 517.27	.05	332
		10, 5, 5← 9, 6, 4	Ground							14 518.96	.05	332
		10, 2, 8←10, 1, 9	Ground							57 887.28	.05	356
		10, 2, 8←10, 1, 9	Ground							57 888.07	.05	356
		10, 2, 8←10, 1, 9	Ground							57 888.86	.05	356
		10, 3, 7←10, 2, 8	Ground							43 543.45	.05	356
		10, 3, 7←10, 2, 8	Ground							43 544.14	.05	356
		10, 3, 7←10, 2, 8	Ground							43 544.84	.05	356
		10, 4, 6←10, 3, 7	Ground							63 236.56	.05	356
		10, 4, 6←10, 3, 7	Ground							63 237.73	.05	356
		10, 4, 6←10, 3, 7	Ground							63 238.90	.05	356
		11, 2,10←10, 3, 7	Ground							41 529.13	.05	356
		11, 2,10←10, 3, 7	Ground							41 530.31	.05	356
		11, 2,10←10, 3, 7	Ground							41 531.49	.05	356
		11, 3, 8←11, 2, 9	Ground							47 653.80	.05	356
		11, 3, 8←11, 2, 9	Ground							47 654.47	.05	356
		11, 3, 8←11, 2, 9	Ground							47 655.14	.05	356
		11, 4, 7←11, 3, 8	Ground							59 181.48	.05	356
		11, 4, 7←11, 3, 8	Ground							59 182.54	.05	356
		11, 4, 7←11, 3, 8	Ground							59 183.59	.05	356
		12, 2,11←11, 3, 8	Ground							36 258.98	.05	356
		12, 2,11←11, 3, 8	Ground							36 260.33	.05	356
		12, 2,11←11, 3, 8	Ground							36 261.67	.05	356
		12, 3, 9←12, 2,10	Ground							54 439.22	.05	356
		12, 3, 9←12, 2,10	Ground							54 439.92	.05	356
		12, 3, 9←12, 2,10	Ground							54 440.61	.05	356
		12, 4, 8←12, 3, 9	Ground							56 285.75	.05	356
		12, 4, 8←12, 3, 9	Ground							56 286.69	.05	356

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2S^{32}$	601	12, 4, 8←12, 3, 9	Ground							56 287.63	.05	356
		13, 2,12←12, 3, 9	Ground							28 278.31	.05	356
		13, 2,12←12, 3, 9	Ground							28 279.87	.05	356
		13, 2,12←12, 3, 9	Ground							28 281.45	.05	356
		14, 2,13←13, 3,10	Ground							18 199.20	.05	356
		14, 2,13←13, 3,10	Ground							18 201.03	.05	356
		14, 2,13←13, 3,10	Ground							18 202.86	.05	356
$(C^{12}H_3)_2S^{34}$	602	1, 1, 1← 0, 0, 0	Ground							23 073.35	.05	332
		1, 1, 0← 1, 0, 1	Ground							11 724.09	.05	332
		2, 1, 1← 2, 0, 2	Ground							13 933.60	.05	332
		3, 1, 2← 3, 0, 3	Ground							17 697.30	.05	332
$C^{13}H_3S^{32}C^{12}H_3$	603	1, 1, 1← 0, 0, 0	Ground							23 192.10	.05	332
		1, 1, 0← 1, 0, 1	Ground							12 032.78	.05	332
		2, 1, 1← 2, 0, 2	Ground							14 090.96	.05	332
		3, 1, 2← 3, 0, 3	Ground							17 569.40	.05	332
s-$C^{12}H_2DS^{32}C^{12}H_3$	604	1, 1, 1← 0, 0, 0	Ground							23 196.66	.05	332
		1, 1, 0← 1, 0, 1	Ground							12 393.28	.05	332
		2, 0, 2← 1, 1, 1	Ground							14 035.40	.05	332
		2, 1, 1← 2, 0, 2	Ground							14 240.30	.05	332
		3, 1, 2← 3, 0, 3	Ground							17 327.39	.05	332
		4, 1, 3← 4, 0, 4	Ground							21 947.29	.05	332
a-$C^{12}H_2DS^{32}C^{12}H_3$	605	1, 1, 1← 0, 0, 0	Ground							22 069.05	.05	332
		1, 1, 0← 1, 0, 1	Ground							11 044.96	.05	332
		2, 0, 2← 1, 1, 1	Ground							16 228.21	.05	332
		2, 1, 1← 2, 0, 2	Ground							13 112.72	.05	332
		3, 1, 2← 3, 0, 3	Ground							16 633.37	.05	332
		4, 1, 3← 4, 0, 4	Ground							21 942.79	.05	332
$C^{12}H_3S^{32}C^{12}D_3$	606	1, 1, 1← 0, 0, 0	Ground	A						20 547.20	.05	332
		1, 1, 1← 0, 0, 0	Ground	A	0					20 547.90	.05	332
		1, 1, 1← 0, 0, 0	Ground	E						20 553.47	.05	332
		1, 1, 0← 1, 0, 1	Ground	A	0					10 413.11	.05	332
		1, 1, 0← 1, 0, 1	Ground	A						10 425.98	.05	332
		1, 1, 0← 1, 0, 1	Ground	A						10 432.81	.05	332
		1, 1, 0← 1, 0, 1	Ground	E						10 441.92	.05	332
		2, 0, 2← 1, 1, 1	Ground	A	0					14 261.38	.05	332
		2, 1, 1← 2, 0, 2	Ground	A						12 111.96	.05	332
		2, 1, 1← 2, 0, 2	Ground	A						12 114.76	.05	332
		2, 1, 1← 2, 0, 2	Ground	A	0					12 122.46	.05	332
		2, 1, 1← 2, 0, 2	Ground	E						12 123.88	.05	332
		3, 1, 2← 3, 0, 3	Ground	A						14 943.65	.05	332
		3, 1, 2← 3, 0, 3	Ground	A						14 949.04	.05	332
		3, 1, 2← 3, 0, 3	Ground	E						14 954.42	.05	332
		3, 1, 2← 3, 0, 3	Ground	A	0					15 001.68	.05	332
		4, 1, 3← 4, 0, 4	Ground	A						19 190.49	.05	332
		4, 1, 3← 4, 0, 4	Ground	E						19 204.21	.05	332
		4, 1, 3← 4, 0, 4	Ground	A						19 206.75	.05	332
		4, 1, 3← 4, 0, 4	Ground	E	0					19 327.03	.05	332
		4, 1, 3← 4, 0, 4	Ground	A	0					19 327.31	.05	332
		5, 1, 4← 5, 0, 5	Ground	A						25 040.66	.05	332
		5, 1, 4← 5, 0, 5	Ground	A	0					25 249.00	.05	332

Ethenylsilane; Ethylene Silane; Ethenesilicane

C_2H_6Si $C_s(C_s,C_{3v})$ $CH_2{:}CHSiH_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$Si^{28}H_3C^{12}H{:}C^{12}H_2$	C_s	611	34 159. M	5 275.20 M	4 820.80 M				
$Si^{28}D_3C^{12}H{:}C^{12}H_2$	C_s	612	24 703.00 M	4 773.26 M	4 404.48 M				
$Si^{29}H_3C^{12}H{:}C^{12}H_2$	C_s	613		5 214.40 M	4 769.61 M				
$Si^{30}H_3C^{12}H{:}C^{12}H_2$	C_s	614		5 156.96 M	4 721.31 M				
$Si^{28}H_3C^{13}H{:}C^{12}H_2$	C_s	615		5 249.80 M	4 787.15 M				
$Si^{28}H_3C^{12}D{:}C^{12}H_2$	C_s	616		5 232.29 M	4 673.35 M				
c-$Si^{28}H_3C^{12}H{:}C^{12}HD$	C_s	617		5 137.09 M	4 625.41 M				
t-$Si^{28}H_3C^{12}H{:}C^{12}HD$	C_s	618		4 888.84 M	4 496.24 M				
s-$Si^{28}H_2DC^{12}H{:}C^{12}H_2$	C_s	619		5 214.80 M	4 666.31 M				
a-$Si^{28}H_2DC^{12}H{:}C^{12}H_2$	C_1	621		5 035.33 M	4 669.87 M				
s-$Si^{28}HD_2C^{12}H{:}C^{12}H_2$	C_s	622		4 815.64 M	4 539.21 M				
a-$Si^{28}HD_2C^{12}H{:}C^{12}H_2$	C_1	623		4 984.80 M	4 526.28 M				
$Si^{28}H_3C^{12}H{:}C^{13}H_2$	C_s	624		5 114.83 M	4 682.70 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
611	0.648 M	0.133 M	0. X		1500	30					

References:

ABC: 331 D_J: D_{JK}: κ: Δ:

μ: 331 eQq: V: 331 I: ω:

Coupling Parameter, $I_\alpha = 5.7923$ amu Å^2. Ref: 331.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$Si^{28}H_3C^{12}H{:}C^{12}H_2$	611	1, 0, 1← 0, 0, 0	Ground	A	1					10 089.96	.05	331
		1, 0, 1← 0, 0, 0	Ground	E	1					10 090.73	.05	331
		1, 0, 1← 0, 0, 0	Ground							10 095.99	.05	331
		1, 1, 0← 1, 0, 1	Ground	E	0					29 337.	10.	331
		1, 1, 0← 1, 0, 1	Ground	A	0					29 343.	10.	331
		2, 0, 2← 1, 0, 1	Ground	A	1					20 174.75	.05	331
		2, 0, 2← 1, 0, 1	Ground	E	1					20 176.20	.05	331
		2, 0, 2← 1, 0, 1	Ground							20 186.62	.05	331
		2, 1, 1← 1, 1, 0	Ground	E	1					20 508.5	.05	331
		2, 1, 1← 1, 1, 0	Ground	A	1					20 621.8	.05	331
		2, 1, 1← 1, 1, 0	Ground							20 646.43	.05	331
		2, 1, 2← 1, 1, 1	Ground							19 737.64	.05	331
		2, 1, 2← 1, 1, 1	Ground	A	1					19 738.6	.05	331
		2, 1, 2← 1, 1, 1	Ground	E	1					19 853.9	.05	331
		2, 1, 1← 2, 0, 2	Ground	E	0					29 784.	10.	331
		2, 1, 1← 2, 0, 2	Ground	A	0					29 789.	10.	331
		7, 1, 6← 7, 1, 7	Ground	E	0					12 714.59	.05	331
		7, 1, 6← 7, 1, 7	Ground	A	0					12 715.13	.05	331
		8, 1, 7← 8, 1, 8	Ground	E	0					16 338.77	.05	331
		8, 1, 7← 8, 1, 8	Ground	A	0					16 339.47	.05	331
		9, 1, 8← 9, 1, 9	Ground	E	0					20 408.43	.05	331
		9, 1, 8← 9, 1, 9	Ground	A	0					20 409.38	.05	331
		10, 1, 9←10, 1,10	Ground	E	0					24 919.07	.05	331
		10, 1, 9←10, 1,10	Ground	A	0					24 920.20	.05	331
$Si^{28}D_3C^{12}H{:}C^{12}H_2$	612	1, 0, 1← 0, 0, 0	Ground	A	1					9 174.9	.05	331
		1, 0, 1← 0, 0, 0	Ground							9 177.78	.05	331
		1, 1, 0← 1, 0, 1	Ground							20 298.50	.05	331
		2, 0, 2← 1, 0, 1	Ground	A	1					18 344.93	.05	331
		2, 0, 2← 1, 0, 1	Ground							18 350.34	.05	331
		2, 1, 1← 1, 1, 0	Ground	E	1					18 701.20	.05	331
		2, 1, 1← 1, 1, 0	Ground	A	1					18 702.11	.05	331
		2, 1, 1← 1, 1, 0	Ground							18 724.23	.05	331
		2, 1, 2← 1, 1, 0	Ground	A	1					17 996.71	.05	331
		2, 1, 2← 1, 1, 0	Ground	E	1					17 997.83	.05	331
		2, 1, 2← 1, 1, 1	Ground							17 986.70	.05	331
		2, 1, 1← 2, 0, 2	Ground							20 672.34	.05	331
		3, 1, 2← 3, 0, 3	Ground							21 242.54	.05	331
		4, 1, 3← 4, 0, 4	Ground							22 020.31	.05	331
$Si^{29}H_3C^{12}H{:}C^{12}H_2$	613	2, 0, 2← 1, 0, 1	Ground							19 962.92	.10	331
		2, 1, 1← 1, 1, 0	Ground							20 412.81	.10	331
		2, 1, 2← 1, 1, 1	Ground							19 523.22	.10	331
$Si^{30}H_3C^{12}H{:}C^{12}H_2$	614	2, 0, 2← 1, 0, 1	Ground							19 751.60	.10	331
		2, 1, 1← 1, 1, 0	Ground							20 192.25	.10	331
		2, 1, 2← 1, 1, 1	Ground							19 320.91	.10	331
$Si^{28}H_3C^{13}H{:}C^{12}H_2$	615	2, 0, 2← 1, 0, 1	Ground							20 067.88	.10	331
		2, 1, 1← 1, 1, 0	Ground							20 536.54	.10	331
		2, 1, 2← 1, 1, 1	Ground							19 611.24	.10	331

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$Si^{28}H_3C^{12}D:C^{12}H_2$	616	2, 0, 2← 1, 0, 1	Ground						19 801.56	.10	331
		2, 1, 1← 1, 1, 0	Ground						20 370.22	.10	331
		2, 1, 2← 1, 1, 1	Ground						19 252.34	.10	331
c-$Si^{28}H_3C^{12}H:C^{12}HD$	617	2, 0, 2← 1, 0, 1	Ground						19 517.07	.10	331
		2, 1, 1← 1, 1, 0	Ground						20 036.68	.10	331
		2, 1, 2← 1, 1, 1	Ground						19 013.32	.10	331
t-$Si^{28}H_3C^{12}H:C^{12}HD$	618	2, 0, 2← 1, 0, 1	Ground						18 766.27	.10	331
		2, 1, 1← 1, 1, 0	Ground						19 162.76	.10	331
		2, 1, 2← 1, 1, 1	Ground						18 377.57	.10	331
s-$Si^{28}H_2DC^{12}H:C^{12}H_2$	619	1, 1, 0← 0, 0, 0	Ground						9 881.05	.10	331
		2, 0, 2← 1, 0, 1	Ground						19 752.92	.10	331
		2, 1, 1← 1, 1, 0	Ground						20 310.72	.10	331
		2, 1, 2← 1, 1, 1	Ground						19 213.72	.10	331
a-$Si^{28}H_2DC^{12}H:C^{12}H_2$	621	1, 1, 0← 0, 0, 0	Ground						9 705.16	.10	331
		2, 0, 2← 1, 0, 1	Ground						19 406.68	.10	331
		2, 1, 1← 1, 1, 0	Ground						19 775.85	.10	331
		2, 1, 2← 1, 1, 1	Ground						19 044.95	.10	331
s-$Si^{28}HD_2C^{12}H:C^{12}H_2$	622	1, 1, 0← 0, 0, 0	Ground						9 354.8	.10	331
		2, 0, 2← 1, 0, 1	Ground						18 707.1	.10	331
		2, 1, 1← 1, 1, 0	Ground						18 986.14	.10	331
		2, 1, 2← 1, 1, 1	Ground						18 433.27	.10	331
a-$Si^{28}HD_2C^{12}H:C^{12}H_2$	623	1, 1, 0← 0, 0, 0	Ground						9 511.02	.10	331
		2, 0, 2← 1, 0, 1	Ground						19 015.05	.10	331
		2, 1, 1← 1, 1, 0	Ground						19 480.67	.10	331
		2, 1, 2← 1, 1, 1	Ground						18 563.63	.10	331
$Si^{28}H_3C^{12}H:C^{13}H_2$	624	2, 0, 2← 1, 0, 1	Ground						19 590.25	.10	331
		2, 1, 1← 1, 1, 0	Ground						20 027.20	.10	331
		2, 1, 2← 1, 1, 1	Ground						19 162.94	.10	331

C_2H_7N $C_s(C_{3v},C_{2v},C_s)$ $C_2H_5NH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$N^{14}H_2C_2^{12}H_5$	C_s	631							

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
631	1.22 T		0. X		3500						

References:

ABC: D_J: D_{JK}: κ: Δ:

μ: 367 eQq: V: 113 I: ω:

Ethylamine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$N^{14}H_2C_2^{12}H_5$	631	Not Reported	Ground						22 130.04	.2	94
		Not Reported	Ground						22 564.05	.2	94
		Not Reported	Ground						22 603.51	.2	94
		Not Reported	Ground						22 618.89	.2	94
		Not Reported	Ground						22 625.17	.2	94
		Not Reported	Ground						22 635.94	.2	94
		Not Reported	Ground						22 641.95	.2	94
		Not Reported	Ground						22 668.35	.2	94
		Not Reported	Ground						22 751.86	.2	94
		Not Reported	Ground						22 789.47	.2	94
		Not Reported	Ground						22 815.64	.2	94
		Not Reported	Ground						22 909.23	.2	94
		Not Reported	Ground						22 975.73	.2	94
		Not Reported	Ground						23 033.75	.2	94
		Not Reported	Ground						23 045.44	.2	94
		Not Reported	Ground						23 196.14	.2	94
		Not Reported	Ground						24 261.72	.2	94
		Not Reported	Ground						23 264.16	.2	94
		Not Reported	Ground						24 291.18	.2	94
		Not Reported	Ground						24 418.80	.2	94
		Not Reported	Ground						24 695.13	.2	94
		Not Reported	Ground						24 802.94	.2	94
		Not Reported	Ground						25 328.64	.2	94

C_2H_8Si $C_{2v}(C_{3v},C_{3v},C_{2v})$ $(CH_3)_2SiH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_2Si^{28}H_2$	C_{2v}	641	16 754.24 M	5 945.44 M	4 896.50 M				
$C^{12}H_3C^{12}D_3Si^{28}H_2$	C_s	642	14 740.79 M	5 198.82 M	4 342.47 M				
$(C^{12}H_3)_2Si^{28}D_2$	C_{2v}	643	13 716.25 M	5 749.07 M	4 722.39 M				
$(C^{12}H_3)_2Si^{29}H_2$	C_{2v}	644	16 606.85 M	5 945.56 M	4 883.83 M				
$(C^{12}H_3)_2Si^{30}H_2$	C_{2v}	645	16 467.26 M	5 945.50 M	4 871.52 M				
$C^{13}H_3C^{12}H_3Si^{28}H_2$	C_s	646	16 605.08 M	5 785.65 M	4 775.22 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
641	0. X	0.75 M	0. X		1649	3					
642					1647	3					
643					1646	3					

References:

ABC: 333 D_J: D_{JK}: κ: Δ:

μ: 333 eQq: V: 333 I: ω:

Add. Refs.: 209, 262, 287

Coupling parameters listed for the following species: 641: $I_\alpha = 3.1635$ amu Å^2; 642: $I_\alpha = 3.1635$ for CH_3 group and $I_\alpha = 6.3221$ for CD_3 group; 643: $I_\alpha = 3.1635$. Ref: 333.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2Si^{28}H_2$	641	1, 1, 1← 0, 0, 0	Ground	AE+EA 0					21 649.82	.05	333
		1, 1, 1← 0, 0, 0	Ground	EE 0					21 651.08	.05	333
		1, 1, 1← 0, 0, 0	Ground	AA 0					21 652.35	.05	333
		1, 1, 0← 1, 0, 1	Ground	AE+EA 0					11 857.06	.05	333
		1, 1, 0← 1, 0, 1	Ground	EE 0					11 858.19	.05	333
		1, 1, 0← 1, 0, 1	Ground	AA 0					11 859.33	.05	333
		2, 1, 1← 2, 0, 2	Ground	AE+EA 0					12 978.49	.05	333
		2, 1, 1← 2, 0, 2	Ground	EE 0					12 979.76	.05	333
		2, 1, 1← 2, 0, 2	Ground	AA 0					12 981.03	.05	333
		3, 0, 3← 2, 1, 2	Ground	AA 0					22 402.03	.05	333
		3, 0, 3← 2, 1, 2	Ground	EE 0					22 402.90	.05	333
		3, 0, 3← 2, 1, 2	Ground	AE+EA 0					22 403.80	.05	333
		3, 1, 2← 3, 0, 3	Ground	AE+EA 0					14 792.71	.05	333
		3, 1, 2← 3, 0, 3	Ground	EE 0					14 794.11	.05	333
		3, 1, 2← 3, 0, 3	Ground	AA 0					14 795.50	.05	333
		4, 1, 3← 4, 0, 4	Ground	AE+EA 0					17 441.16	.05	333
		4, 1, 3← 4, 0, 4	Ground	EE 0					17 442.72	.05	333
		4, 1, 3← 4, 0, 4	Ground	AA 0					17 444.27	.05	333
		5, 1, 4← 5, 0, 5	Ground	AE+EA 0					21 068.32	.05	333
		5, 1, 4← 5, 0, 5	Ground	EE 0					21 070.13	.05	333
		5, 1, 4← 5, 0, 5	Ground	AA 0					21 071.97	.05	333
		6, 1, 5← 6, 0, 6	Ground	AE+EA 0					25 771.55	.05	333
		6, 1, 5← 6, 0, 6	Ground	EE 0					25 773.65	.05	333
		6, 1, 5← 6, 0, 6	Ground	AA 0					25 775.75	.05	333
$C^{12}H_3C^{12}D_3Si^{28}H_2$	642	1, 1, 1← 0, 0, 0	Ground	E 0					19 082.67	.05	333
		1, 1, 1← 0, 0, 0	Ground	A 0					19 083.52	.05	333
		1, 1, 0← 1, 0, 1	Ground	E 0					10 397.79	.05	333
		1, 1, 0← 1, 0, 1	Ground	A 0					10 398.58	.05	333
		2, 1, 1← 2, 0, 2	Ground	E 0					11 309.18	.05	333
		2, 1, 1← 2, 0, 2	Ground	A 0					11 310.02	.05	333
		3, 0, 3← 2, 1, 2	Ground	A 0					19 663.69	.05	333
		3, 0, 3← 2, 1, 2	Ground	E 0					19 664.24	.05	333
		3, 1, 2← 3, 0, 3	Ground	E 0					12 776.79	.05	333
		3, 1, 2← 3, 0, 3	Ground	A 0					12 777.78	.05	333
		4, 1, 3← 4, 0, 4	Ground	E 0					14 909.62	.05	333
		4, 1, 3← 4, 0, 4	Ground	A 0					14 910.75	.05	333
		5, 1, 4← 5, 0, 5	Ground	E 0					17 823.41	.05	333
		5, 1, 4← 5, 0, 5	Ground	A 0					17 824.74	.05	333
		5, 2, 3← 5, 1, 4	Ground	E 0					25 590.10		262
		5, 2, 3← 5, 1, 4	Ground	A 0					25 592.00		262
		6, 1, 5← 6, 0, 6	Ground	E 0					21 604.75	.05	333
		6, 1, 5← 6, 0, 6	Ground	A 0					21 606.33	.05	333
		6, 2, 4← 6, 1, 5	Ground	E 0					24 994.91		262
		6, 2, 4← 6, 1, 5	Ground	A 0					24 996.80		262
$(C^{12}H_3)_2Si^{28}D_2$	643	1, 1, 1← 0, 0, 0	Ground	AE+EA 0					18 438.12	.05	333
		1, 1, 1← 0, 0, 0	Ground	EE 0					18 438.86	.05	333
		1, 1, 1← 0, 0, 0	Ground	AA 0					18 439.63	.05	333
		1, 1, 0← 1, 0, 1	Ground	AE+EA 0					8 993.41	.05	333
		1, 1, 0← 1, 0, 1	Ground	EE 0					8 994.12	.05	333
		1, 1, 0← 1, 0, 1	Ground	AA 0					8 994.82	.05	333

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2Si^{28}D_2$	643	2, 1, 1← 2, 0, 2	Ground	AE+EA 0					10 112.93	.05	333
		2, 1, 1← 2, 0, 2	Ground	EE 0					10 113.72	.05	333
		2, 1, 1← 2, 0, 2	Ground	AA 0					10 114.53	.05	333
		3, 0, 3← 2, 1, 2	Ground	AA 0					24 012.43	.05	333
		3, 0, 3← 2, 1, 2	Ground	EE 0					24 012.92	.05	333
		3, 0, 3← 2, 1, 2	Ground	AE+EA 0					24 013.39	.05	333
		3, 1, 2← 3, 0, 3	Ground	AE+EA 0					11 958.60	.05	333
		3, 1, 2← 3, 0, 3	Ground	EE 0					11 959.51	.05	333
		3, 1, 2← 3, 0, 3	Ground	AA 0					11 960.42	.05	333
		4, 1, 3← 4, 0, 4	Ground	AE+EA 0					14 695.69	.05	333
		4, 1, 3← 4, 0, 4	Ground	EE 0					14 695.75	.05	333
		4, 1, 3← 4, 0, 4	Ground	AA 0					14 697.84	.05	333
		5, 1, 4← 5, 0, 5	Ground	AE+EA 0					18 462.82	.05	333
		5, 1, 4← 5, 0, 5	Ground	EE 0					18 464.11	.05	333
		5, 1, 4← 5, 0, 5	Ground	AA 0					18 465.35	.05	333
$(C^{12}H_3)_2Si^{29}H_2$	644	1, 1, 1← 0, 0, 0	Ground	AE+EA 0					21 489.88	.20	333
		1, 1, 1← 0, 0, 0	Ground	EE 0					21 491.07	.20	333
		1, 1, 1← 0, 0, 0	Ground	AA 0					21 492.33	.20	333
		4, 1, 3← 4, 0, 4	Ground	AE+EA 0					17 394.96	.20	333
		4, 1, 3← 4, 0, 4	Ground	EE 0					17 396.51	.20	333
		4, 1, 3← 4, 0, 4	Ground	AA 0					17 398.06	.20	333
		5, 1, 4← 5, 0, 5	Ground	AE+EA 0					21 086.34	.20	333
		5, 1, 4← 5, 0, 5	Ground	EE 0					21 088.16	.20	333
		5, 1, 4← 5, 0, 5	Ground	AA 0					21 089.93	.20	333
$(C^{12}H_3)_2Si^{30}H_2$	645	1, 1, 1← 0, 0, 0	Ground	AE+EA 0					21 337.99	.20	333
		1, 1, 1← 0, 0, 0	Ground	EE 0					21 339.18	.20	333
		1, 1, 1← 0, 0, 0	Ground	AA 0					21 340.20	.20	333
		4, 1, 3← 4, 0, 4	Ground	AE+EA 0					17 353.41	.20	333
		4, 1, 3← 4, 0, 4	Ground	EE 0					17 354.68	.20	333
		4, 1, 3← 4, 0, 4	Ground	AA 0					17 356.26	.20	333
		5, 1, 4← 5, 0, 5	Ground	AE+EA 0					21 106.76	.20	333
		5, 1, 4← 5, 0, 5	Ground	EE 0					21 108.42	.20	333
		5, 1, 4← 5, 0, 5	Ground	AA 0					21 110.22	.20	333
$C^{13}H_3C^{12}H_3Si^{28}H_2$	646	1, 1, 1← 0, 0, 0	Ground	AE+EA 0					21 379.40	.20	333
		1, 1, 1← 0, 0, 0	Ground	EE 0					21 380.70	.20	333
		1, 1, 1← 0, 0, 0	Ground	AA 0					21 382.00	.20	333
		4, 1, 3← 4, 0, 4	Ground	AE+EA 0					17 180.01	.20	333
		4, 1, 3← 4, 0, 4	Ground	EE 0					17 181.68	.20	333
		4, 1, 3← 4, 0, 4	Ground	AA 0					17 183.30	.20	333
		5, 1, 4← 5, 0, 5	Ground	AE+EA 0					20 646.21	.20	333
		5, 1, 4← 5, 0, 5	Ground	EE 0					20 647.95	.20	333
		5, 1, 4← 5, 0, 5	Ground	AA 0					20 649.83	.20	333
		6, 1, 5← 6, 0, 6	Ground	AE+EA 0					24 142.60	.20	333
		6, 1, 5← 6, 0, 6	Ground	EE 0					25 144.60	.20	333
		6, 1, 5← 6, 0, 6	Ground	AA 0					25 146.60	.20	333

650 - Ethylsilane
Ethylsilicane

Molecular Constant Table

C_2H_8Si $C_s(C_{3v},C_s,C_{3v})$ $CH_3CH_2SiH_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2Si^bH_3$	C_s	651							

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
651	0.72 M	0.36 M	0. X		1940	40					

References:

ABC: D_J: D_{JK}: κ: Δ:

μ: 306 eQq: V: 306, I: ω:

No spectral lines

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660 - Trifluoroacetic Acid-Formic Acid Complex

Molecular Constant Table

$C_3H_3F_3O_4$ $CF_3COOH{\cdot}HCOOH$

B + C = 1154.4 MHz. Ref: 316.

Trifluoroacetic Acid-Formic Acid Complex

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}F_3^{19}C^{12}O^{16}O^{16}H{\cdot}HC^{12}O^{16}O^{16}H$	661	3, , ← 2, ,	Ground						3 462.2		316
		7, , ← 6, ,	Ground						8 079.1		316
		8, , ← 7, ,	Ground						9 235.2		316
		9, , ← 8, ,	Ground						10 388.5		316
		16, , ←15, ,	Ground						18 473.0		316
		17, , ←16, ,	Ground						19 621.8		316
		18, , ←17, ,	Ground						20 779.2		316
		19, , ←18, ,	Ground						21 938.5		316
$C^{12}F_3^{19}C^{12}O^{16}O^{16}D{\cdot}HC^{12}O^{16}O^{16}H$	662	16, , ←15, ,	Ground						18 397.0		343
		19, , ←18, ,	Ground						21 842.7		343
$C^{12}F_3^{19}C^{12}O^{16}O^{16}H{\cdot}HC^{12}O^{16}O^{16}D$	663	16, , ←15, ,	Ground						18 351.7		343
		19, , ←18, ,	Ground						21 794.2		343
$C^{12}F_3^{19}C^{12}O^{16}O^{16}D{\cdot}HC^{12}O^{16}O^{16}D$	664	16, , ←15, ,	Ground						18 270.0		343
		19, , ←18, ,	Ground						21 669.7		343

C_3H_3NO $C_s(C_{3v},C_s)$ CH_3COCN

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}O^{16}C^{12}N^{14}$	C_s	671	10 185.46 M	4 157.53 M	3 002.75 M				2.871
$C^{13}H_3C^{12}O^{16}C^{12}N^{14}$	C_s	672	9 906.07 M	4 105.57 M	2 951.68 M				2.897
$C^{12}H_3C^{12}O^{16}C^{13}N^{14}$	C_s	673	10 184.58 M	4 125.37 M	2 986.21 M				2.890
$C^{12}H_3C^{12}O^{18}C^{12}N^{14}$	C_s	674	9 657.42 M	4 085.73 M	2 918.86 M				2.883
$C^{12}D_3C^{12}O^{16}C^{12}N^{14}$	C_s	675	8 728.40 M	3 875.60 M	2 772.32 M				6.008
$C^{12}D_3C^{13}O^{16}C^{12}N^{14}$	C_s	676	8 722.81 M	3 870.29 M	2 769.23 M				6.021

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
671	2.42 M	2.46 M	0. X		1210	30					
672					1226						
673					1214						
674					1204						

References:

ABC: 246 D_J: D_{JK}: κ: Δ: 246

μ: 246 eQq: V: 288 I: ω:

For all species, the coupling parameter is: $I_\alpha = 3.1421$ amu Å^2. For species 677, $(A-C)/2 = 3545$ MHz. For species 678, $(A-C)/2 = 3235.5$ MHz. For species 679, $(A-C)/2 = 3257.5$ MHz. Ref: 246.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}O^{16}C^{12}N^{14}$	671	1, 1, 1← 0, 0, 0	Ground							13 188.21	.2	246
		2, 0, 2← 1, 0, 1	Ground							14 170.15	.2	246
		2, 0, 2← 1, 1, 1	Ground							8 142.5	.3	246
		2, 1, 2← 1, 0, 1	Ground							19 193.60	.2	246
		2, 1, 1← 1, 1, 0	Ground							15 475.34	.2	246
		2, 1, 2← 1, 1, 1	Ground							13 165.78	.2	246
		3, 0, 3← 2, 0, 2	Ground	E	0					20 894.60	.2	246
		3, 0, 3← 2, 0, 2	Ground	A	0					20 895.08	.2	246
		3, 0, 3← 2, 1, 2	Ground							15 871.37	.2	246
		3, 1, 2← 2, 1, 1	Ground							23 112.13	.2	246
		3, 1, 3← 2, 1, 2	Ground							19 659.98	.2	246
		3, 2, 2← 2, 2, 1	Ground							21 481.42	.2	246
		3, 1, 2← 3, 0, 3	Ground							10 705.27	.2	246
		4, 0, 4← 3, 1, 3	Ground							23 479.26	.2	246
		4, 1, 3← 3, 1, 2	Ground	E	0					30 608.53	.2	246
		4, 1, 3← 3, 1, 2	Ground	A	0					30 610.27	.2	246
		4, 1, 4← 3, 1, 3	Ground							26 064.43	.2	246
		4, 3, 1← 3, 3, 0	Ground							28 981.60	.2	246
		5, 0, 5← 4, 0, 4	Ground							33 344.70	.2	246
		5, 0, 5← 4, 1, 4	Ground							30 759.12	.2	246
		5, 1, 4← 4, 2, 3	Ground	E	1					23 527.46	.2	246
		5, 1, 4← 4, 2, 3	Ground	A	0					23 529.29	.2	246
		5, 2, 3← 5, 1, 4	Ground							16 497.52	.2	246
		6, 1, 5← 6, 0, 6	Ground	E	1					24 205.33	.2	246
		6, 1, 5← 6, 0, 6	Ground	A	1					24 211.49	.2	246
		6, 2, 4← 6, 1, 5	Ground							17 576.96	.2	246
		6, 3, 3← 6, 2, 4	Ground							28 180.80	.2	246
		7, 1, 6← 7, 0, 7	Ground	E	1					30 537.91	.2	246
		7, 1, 6← 7, 0, 7	Ground	A	1					30 545.52	.2	246
		7, 2, 5← 7, 1, 6	Ground	E	1					19 935.72	.2	246
		7, 2, 5← 7, 1, 6	Ground	A	1					19 939.43	.2	246
		7, 3, 4← 7, 2, 5	Ground							26 389.94	.2	246
		8, 2, 6← 8, 1, 7	Ground	E	1					23 711.10	.2	246
		8, 2, 6← 8, 1, 7	Ground	A	1					23 716.83	.2	246
		8, 3, 5← 8, 2, 6	Ground	E	1					25 141.40	.2	246
		8, 3, 5← 8, 2, 6	Ground	A	1					25 142.58	.2	246
		9, 2, 7← 9, 1, 8	Ground	E	1					28 859.57	.2	246
		9, 2, 7← 9, 1, 8	Ground	A	1					28 867.37	.2	246
		9, 3, 6← 9, 2, 7	Ground	E	1					24 899.85	.2	246
		9, 3, 6← 9, 2, 7	Ground	A	1					24 901.87	.2	246
		10, 3, 7←10, 2, 8	Ground	E	1					26 008.42	.2	246
		10, 3, 7←10, 2, 8	Ground	A	1					26 012.18	.2	246
		11, 3, 8←11, 2, 9	Ground	E	0					28 680.63	.2	246
		11, 3, 8←11, 2, 9	Ground	A	0					28 686.62	.2	246
		11, 4, 7←11, 3, 8	Ground							34 771.	.3	246
		12, 3, 9←12, 2,10	Ground	E	0					32 978.82	.2	246
		12, 3, 9←12, 2,10	Ground	A	0					32 987.34	.2	246
		12, 4, 8←12, 3, 9	Ground							33 169.95	.2	246

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{13}H_3C^{12}O^{16}C^{12}N^{14}$	672	1, 1, 1← 0, 0, 0	Ground							12 858.27	.2	246
		2, 0, 2← 1, 0, 1	Ground							13 959.01	.2	246
		2, 1, 2← 1, 0, 1	Ground							18 761.11	.2	246
		2, 1, 1← 1, 1, 0	Ground							15 268.39	.2	246
		2, 1, 2← 1, 1, 1	Ground							12 960.62	.2	246
		3, 1, 3← 2, 0, 2	Ground							24 150.7	.3	246
		4, 0, 4← 3, 0, 3	Ground							26 817.10	.2	246
		4, 1, 4← 3, 0, 3	Ground							29 228.46	.2	246
		4, 1, 4← 3, 1, 3	Ground							25 644.76	.2	246
		4, 2, 2← 3, 2, 1	Ground							29 518.4	.3	246
		5, 0, 5← 4, 0, 4	Ground							32 773.38	.2	246
		7, 3, 4← 7, 2, 5	Ground							25 278.01	.2	246
		8, 2, 6← 8, 1, 7	Ground	E	0					23 536.65	.2	246
		8, 2, 6← 8, 1, 7	Ground	A	0					23 541.99	.2	246
		8, 3, 5← 8, 2, 6	Ground							24 161.20	.2	246
		9, 2, 7← 9, 1, 8	Ground	E	0					28 789.33	.2	246
		9, 2, 7← 9, 1, 8	Ground	A	0					28 796.36	.2	246
		9, 3, 6← 9, 2, 7	Ground							24 109.5	.2	246
		10, 3, 7←10, 2, 8	Ground	E	0					25 448.26	.2	246
		10, 3, 7←10, 2, 8	Ground	A	0					25 452.03	.2	246
		11, 3, 8←11, 2, 9	Ground	E	0					28 375.46	.2	246
		11, 3, 8←11, 2, 9	Ground	A	0					28 381.10	.2	246
		11, 4, 7←11, 3, 8	Ground							33 182.59	.2	246
		12, 3, 9←12, 2,10	Ground	E	0					32 918.68	.2	246
		12, 3, 9←12, 2,10	Ground	A	0					32 927.01	.2	246
$C^{12}H_3C^{12}O^{16}C^{13}N^{14}$	673	1, 1, 1← 0, 0, 0	Ground							13 170.70	.2	246
		2, 0, 2← 1, 0, 1	Ground							14 076.57	.2	246
		2, 1, 2← 1, 0, 1	Ground							19 143.21	.2	246
		2, 1, 1← 1, 1, 0	Ground							15 362.32	.2	246
		2, 1, 2← 1, 1, 1	Ground							13 083.99	.2	246
		3, 1, 3← 2, 0, 2	Ground							24 605.75	.2	246
		3, 1, 2← 2, 1, 1	Ground	E	0					22 945.22	.2	246
		3, 1, 2← 2, 1, 1	Ground	A	0					22 946.19	.2	246
		3, 1, 3← 2, 1, 2	Ground							19 537.93	.2	246
		4, 0, 4← 3, 0, 3	Ground							27 110.93	.2	246
		4, 0, 4← 3, 1, 3	Ground							23 270.4	.4	246
		4, 1, 4← 3, 0, 3	Ground							29 478.10	.2	246
		4, 1, 3← 3, 1, 2	Ground							30 394.56	.2	246
		4, 1, 4← 3, 1, 3	Ground							25 907.24	.2	246
		4, 2, 3← 3, 2, 2	Ground							28 332.05	.2	246
		5, 0, 5← 4, 0, 4	Ground							33 161.23	.2	246
		5, 0, 5← 4, 1, 4	Ground							30 524.12	.2	246
		5, 1, 5← 4, 1, 4	Ground							32 181.45	.2	246
		6, 3, 3← 6, 2, 4	Ground							28 389.86	.2	246
		7, 2, 5← 7, 1, 6	Ground	E	0					19 824.98	.2	246
		7, 2, 5← 7, 1, 6	Ground	A	0					19 828.54	.2	246
		7, 3, 4← 7, 2, 5	Ground							26 593.24	.2	246
		8, 2, 6← 8, 1, 7	Ground	E	0					23 487.74	.2	246
		8, 2, 6← 8, 1, 7	Ground	A	0					23 492.79	.2	246
		8, 3, 5← 8, 2, 6	Ground	E	0					25 299.99	.2	246

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_i'	F'	F_i	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H\ C^{12}O^{16}C^{13}N^{14}$	673	8, 3, 5← 8, 2, 6	Ground	A	0					25 301.05	.2	246
		9, 2, 7← 9, 1, 8	Ground	E	0					28 513.87	.2	246
		9, 2, 7← 9, 1, 8	Ground	A	0					28 521.60	.2	246
		9, 3, 6← 9, 2, 7	Ground	E	0					24 971.91	.2	246
		9, 3, 6← 9, 2, 7	Ground	A	0					24 973.89	.2	246
		10, 3, 7←10, 2, 8	Ground	E	0					25 954.59	.2	246
		10, 3, 7←10, 2, 8	Ground	A	0					25 958.15	.2	246
		11, 3, 8←11, 2, 9	Ground	E	0					28 467.34	.2	246
		11, 3, 8←11, 2, 9	Ground	A	0					28 473.03	.2	246
		12, 3, 9←12, 2,10	Ground	E	0					32 586.38	.2	246
		12, 3, 9←12, 2,10	Ground	A	0					32 594.33	.2	246
		12, 4, 8←12, 3, 9	Ground							33 415.93	.2	246
$C^{12}H_3C^{12}O^{18}C^{12}N^{14}$	674	1, 1, 1← 0, 0, 0	Ground							12 577.	2.	246
		2, 0, 2← 1, 0, 1	Ground							13 844.50	.2	246
		2, 1, 2← 1, 0, 1	Ground							18 414.00	.2	246
		2, 1, 1← 1, 1, 0	Ground							15 176.04	.2	246
		2, 1, 2← 1, 1, 1	Ground							12 842.31	.2	246
		3, 1, 3← 2, 0, 2	Ground							23 733.95	.2	246
		4, 0, 4← 3, 1, 3	Ground							23 174.95	.2	246
		4, 1, 4← 3, 1, 3	Ground							25 392.84	.2	246
		5, 0, 5← 4, 1, 4	Ground							30 186.53	.2	246
		5, 1, 5← 4, 1, 4	Ground							31 519.18	.2	246
		6, 3, 3← 6, 2, 4	Ground	A	0					25 774.16	.2	246
		6, 3, 3← 6, 2, 4	Ground	E	0					25 775.01	.2	246
		7, 3, 4← 7, 2, 5	Ground							24 132.67	.2	246
		8, 2, 6← 8, 1, 7	Ground	E	0					23 607.22	.2	246
		8, 2, 6← 8, 1, 7	Ground	A	0					23 612.92	.2	246
		8, 3, 5← 8, 2, 6	Ground							23 191.46	.2	246
		9, 6← 9, 2, 7	Ground							23 401.52	.2	246
		9, 3, 6← 9, 2, 7	Ground	A	0					23 403.71	.2	246
		10, 3, 7←10, 2, 8	Ground	E	0					25 076.08	.2	246
		10, 3, 7←10, 2, 8	Ground	A	0					25 080.16	.2	246
		11, 4, 7←11, 3, 8	Ground							31 542.42	.2	246
		12, 4, 8←12, 3, 9	Ground							30 531.92	.2	246
$C^{12}D_3C^{12}O^{16}C^{12}N^{14}$	675	1, 1, 1← 0, 0 0	Ground							11 500.72	.3	246
		2, 0, 2← 1, 0, 1	Ground							13 128.25	.2	246
		2, 1, 2← 1, 0, 1	Ground							17 046.5	.5	246
		2, 1, 1← 1, 1, 0	Ground							14 399.12	.2	246
		2, 1, 2← 1, 1, 1	Ground							12 192.56	.2	246
		3, 0, 3← 2, 0, 2	Ground							19 297.8	.3	246
		3, 1, 2← 2, 1, 1	Ground							21 484.8	.3	246
		4, 0, 4← 3, 0, 3	Ground							25 106.62	.2	246
		4, 0, 4← 3, 1, 3	Ground							22 297.6	.2	246
		4, 1, 4← 3, 0, 3	Ground							26 903.58	.2	246
		4, 1, 3← 3, 1, 2	Ground							28 410.93	.2	246
		4, 1, 4← 3, 1, 3	Ground							24 093.70	.2	246
		4, 2, 3← 3, 2, 2	Ground							26 461.42	.2	246
		5, 1, 5← 4, 0, 4	Ground							31 690.10	.2	246
		5, 1, 5← 4, 1, 4	Ground							29 895.95	.3	246

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}D_3C^{12}O^{16}C^{12}N^{14}$	675	5, 2, 4← 4, 2, 3	Ground						32 867.29	.2	246
		5, 3, 2← 5, 2, 3	Ground						23 897.3	.2	246
		6, 2, 4← 6, 1, 5	Ground						15 192.6	.2	246
		7, 2, 5← 7, 1, 6	Ground						17 969.7	.2	246
		8, 3, 5← 8, 2, 6	Ground						20 267.8	.2	246
		9, 3, 6← 9, 2, 7	Ground						20 873.53	.2	246
		9, 4, 5← 9, 3, 6	Ground						30 889.66	.2	246
		10, 3, 7←10, 2, 8	Ground						22 933.80	.2	246
		10, 4, 6←10, 3, 7	Ground						28 695.97	.2	246
		11, 3, 8←11, 2, 9	Ground						26 550.51	.2	246
		12, 4, 8←12, 3, 9	Ground						26 781.28	.2	246
$C^{12}D_3C^{13}O^{16}C^{12}N^{14}$	676	1, 1, 1← 0, 0, 0	Ground						11 492.04	.2	246
		2, 1, 2← 1, 0, 1	Ground						17 030.50	.2	246
		2, 1, 1← 1, 1, 0	Ground						14 380.50	.2	246
		2, 1, 2← 1, 1, 1	Ground						12 177.98	.2	246
		4, 0, 4← 3, 0, 3	Ground						25 076.94	.2	246
		4, 1, 4← 3, 0, 3	Ground						26 877.25	.2	246
		4, 1, 4← 3, 1, 3	Ground						24 065.46	.2	246
		4, 2, 3← 3, 2, 2	Ground						26 427.20	.2	246
		5, 2, 4← 4, 2, 3	Ground						32 826 45	.2	246
		5, 3, 2← 5, 2, 3	Ground						23 888.35	.2	246
		10, 3, 7←10, 2, 8	Ground						22 907.56	.2	246
		10, 4, 6←10, 3, 7	Ground						28 705.21	.2	246
		11, 3, 8←11, 2, 9	Ground						26 507.05	.2	246
		11, 4, 7←11, 3, 8	Ground						27 152.82	.2	246
		12, 4, 8←12, 3, 9	Ground						26 771.04	.2	246
s-$C^{12}H_2DC^{12}O^{16}C^{12}N^{14}$	677	3, 1, 3← 2, 0, 2	Ground						23 976.34	.2	246
		3, 1, 2← 2, 1, 1	Ground						22 174.5	.2	246
		4, 0, 4← 3, 1, 3	Ground						22 417.94	.2	246
		8, 2, 6← 8, 1, 7	Ground						22 617.57	.2	246
		9, 3, 6← 9, 2, 7	Ground						24 655.85	.2	246
a-$C^{12}HD_2C^{12}O^{16}C^{12}N^{14}$	678	6, 1, 5← 6, 0, 6	Ground						22 833.	1.	246
		7, 3, 4← 7, 2, 5	Ground						23 321.5	.2	246
		8, 2, 6← 8, 1, 7	Ground						22 351.7	.2	246
		8, 3, 5← 8, 2, 6	Ground						22 358.8	.2	246
		9, 3, 6← 9, 2, 7	Ground						22 454.2	.2	246
		10, 3, 7←10, 2, 8	Ground						23 897.77	.2	246
		10, 3, 7←10, 2, 8	Ground						23 911.19	.2	246
a-$C^{12}H_2DC^{12}O^{16}C^{12}N^{14}$	679	3, 1, 3← 2, 0, 2	Ground						23 591.75		246
		3, 1, 2← 2, 1, 1	Ground						22 748.5		246
		4, 0, 4← 3, 1, 3	Ground						23 451.09		246
		6, 1, 5← 6, 0, 6	Ground						24 014.94		246
		7, 3, 4← 7, 2, 5	Ground						23 044.93		246
		8, 2, 6← 8, 1, 7	Ground						23 568.45		246
		8, 2, 6← 8, 1, 7	Ground						23 570.53		246
		8, 3, 5← 8, 2, 6	Ground						22 276.07		246
		9, 3, 6← 9, 2, 7	Ground						22 726.47		246
		10, 3, 7←10, 2, 8	Ground						24 691.50		246
		10, 3, 7←10, 2, 8	Ground						24 692.58		246

C_3H_4O $C_s(C_{3v},C_s)$ $CH_3CH{:}CO$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H{:}C^{12}O^{16}$	C_s	681	38 350.[1] M	4 507.40 M	4 136.97 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
681	1.79 M		0. X		1200	10					

1. This constant was calculated assuming $I_\alpha = 3.14$ amu Å^2. Rotational constants were calculated from ν_A values extrapolated to infinite barrier height.

References:

ABC: 341 D_J: D_{JK}: κ: Δ:

μ: 341 eQq: V: 341 I: ω:

Coupling parameter (methyl group): $I_\alpha = 3.14$ amu Å^2. Ref: 341.

Methyl Ketene

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H{:}C^{12}O^{16}$	681	2, 0, 2← 1, 0, 1	Ground	E	0					17 285.1	.1	341
		2, 0, 2← 1, 0, 1	Ground	A	0					17 285.9	.1	341
		2, 1, 1← 1, 1, 0	Ground	E	0					17 621.4	.1	341
		2, 1, 1← 1, 1, 0	Ground	A	0					17 659.9	.1	341
		2, 1, 2← 1, 1, 1	Ground	A	0					16 918.5	.1	341
		2, 1, 2← 1, 1, 1	Ground	E	0					16 955.5	.1	341
		3, 0, 3← 2, 0, 2	Ground	E	0					25 919.8	.1	341
		3, 0, 3← 2, 0, 2	Ground	A	0					25 921.0	.1	341
		3, 1, 2← 2, 1, 1	Ground	E	0					26 474.7	.1	341
		3, 1, 2← 2, 1, 1	Ground	A	0					26 487.7	.1	341
		3, 1, 3← 2, 1, 2	Ground	A	0					25 375.6	.1	341
		3, 1, 3← 2, 1, 2	Ground	E	0					25 386.4	.1	341
		3, 2, ← 2, 2,	Ground	E	0					25 835.2	.1	341 [1]
		3, 2, ← 2, 2,	Ground	E	0					26 023.4	.1	341 [1]
		3, 2, 1← 2, 2, 0	Ground	A	0					25 946.8	.1	341
		3, 2, 2← 2, 2, 1	Ground	A	0					25 934.9	.1	341

[1] Definite assignments for these lines were not given.

C_3H_4O $C_s(C_s,C_s)$ $CH_2{:}CHCHO$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_2{:}C^{12}HC^{12}HO^{16}$	C_s	691		4 659.53 M	4 242.71 M				0.05

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_1	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
691	3.06 M	0.54 M	0. X		5000						

References:
ABC: 198 D_J: D_{JK}: κ: Δ: 198
μ: 198 eQq: V: 198 I: ω:
Add. Ref.: 103

Rotational constants for excited torsional states:
v = 1: B = 4666.19 ± .02 MHz, C = 4259.66 ± .02 MHz
v = 2: B = 4672.10 ± .02 MHz, C = 4273.56 ± .02 MHz
v = 3: B = 4678.69 ± .02 MHz, C = 4290.29 ± .02 MHz.
The torsional frequency is 200 ± 50 cm^{-1}. Ref: 198.

s-trans-Acrolein

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2{:}C^{12}HC^{12}HO^{16}$	691	2, 1, 1← 1, 0, 1	Ground	1					18 258.18		198
		2, 1, 1← 1, 1, 0	Ground	0					18 211.08		198
		3, 0, 3← 2, 0, 2	Ground	0					26 694.37		198
		3, 0, 3← 2, 0, 2	Ground	1					26 765.43		198
		3, 0, 3← 2, 0, 2	Ground	2					26 824.88		198
		3, 0, 3← 2, 0, 2	Ground	3					26 895.18		198
		3, 1, 2← 2, 1, 1	Ground	0					27 329.62		198
		3, 1, 2← 2, 1, 1	Ground	2					27 432.89		198
		3, 1, 2← 2, 1, 1	Ground	3					27 487.70		198
		3, 1, 3← 2, 1, 2	Ground	0					26 079.47		198
		3, 1, 3← 2, 1, 2	Ground	1					26 165.87		198
		3, 1, 3← 2, 1, 2	Ground	3					26 322.50		198
		4, 0, 4← 3, 0, 3	Ground	0					35 577.96		198
		4, 0, 4← 3, 0, 3	Ground	2					35 752.72		198
		4, 0, 4← 3, 0, 3	Ground	3					35 846.64		198
		4, 1, 3← 3, 1, 2	Ground	0					36 436.03		198

C_3H_5F $C_s(C_{3v},C_s,C_s)$ $CH_3CH{:}CHF$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
c-$C^{12}H_3C^{12}H{:}C^{12}HF^{19}$-A	C_s	701	17 830.24 M	5 657.32 M	4 406.91 M				3.013
c-$C^{12}H_3C^{12}H{:}C^{12}HF^{19}$-E	C_s	702	17 824.02 M	5 656.19 M	4 406.79 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
701	1.04 M	1.02 M	0. X		1057	50					

References:

ABC: 342 D_J: D_{JK}: κ: Δ: 342

μ: 342 eQq: V: 342 I: ω:

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
c-$C^{12}H_3C^{12}H{:}C^{12}HF^{19}$-A	701	1, 0, 1← 0, 0, 0		A	0					10 064.23	.2	342
		1, 1, 0← 1, 0, 1		A	0					13 423.33	.2	342
		2, 0, 2← 1, 0, 1		A	0					20 036.82	.2	342
		2, 1, 2← 1, 0, 1		A	0					31 050.39	.2	342
		2, 1, 1← 1, 1, 0		A	0					21 378.87	.2	342
		2, 1, 2← 1, 1, 1		A	0					18 877.93	.2	342
		2, 1, 1← 2, 0, 2		A	0					14 765.85	.2	342
		3, 0, 3← 2, 0, 2		A	0					29 829.55	.2	342
		3, 0, 3← 2, 1, 2		A	0					18 815.98	.2	342
		3, 1, 2← 2, 1, 1		A	0					32 008.80	.2	342
		3, 1, 3← 2, 1, 2		A	0					28 261.19	.2	342
		3, 2, 1← 2, 2, 0		A	0					30 555.37	.2	342
		3, 1, 2← 3, 0, 3		A	0					16 945.20	.2	342
		3, 2, 1← 3, 1, 2		A	0					35 155.36	.2	342
		4, 0, 4← 3, 1, 3		A	0					29 923.74	.2	342
		4, 1, 3← 4, 0, 4		A	0					20 136.88	.2	342
		4, 2, 2← 4, 1, 3		A	0					33 666.44	.2	342
		5, 1, 4← 5, 0, 5		A	0					24 515.44	.2	342
		5, 2, 3← 5, 1, 4		A	0					32 480.24	.2	342
		6, 1, 5← 6, 0, 6		A	0					30 187.73	.2	342
		6, 2, 4← 6, 1, 5		A	0					31 938.43	.2	342
		7, 2, 5← 7, 1, 6		A	0					32 338.71	.2	342
		8, 2, 6← 8, 1, 7		A	0					33 917.68	.2	342
c-$C^{12}H_3C^{12}H{:}C^{12}HF^{19}$-E	702	1, 0, 1← 0, 0, 0		E	0					10 062.98	.2	342
		1, 1, 0← 1, 0, 1		E	0					13 419.40	.2	342
		2, 0, 2← 1, 0, 1		E	0					20 034.48	.2	342
		2, 1, 2← 1, 0, 1		E	0					31 043.76	.2	342
		2, 1, 1← 1, 1, 0		E	0					21 373.90	.2	342
		2, 1, 2← 1, 1, 1		E	0					18 877.90	.2	342
		2, 1, 1← 2, 0, 2		E	0					14 759.00	.2	342
		3, 0, 3← 2, 0, 2		E	0					29 826.39	.2	342
		3, 0, 3← 2, 1, 2		E	0					29 922.74	.2	342
		3, 1, 2← 2, 1, 1		E	0					32 003.26	.2	342
		3, 1, 3← 2, 1, 2		E	0					28 259.80	.2	342
		3, 1, 2← 3, 0, 3		E	0					16 936.38	.2	342
		4, 1, 3← 4, 0, 4		E	0					20 123.76	.2	342
		4, 2, 2← 4, 1, 3		E	0					33 661.10	.2	342
		5, 1, 4← 5, 0, 5		E	0					24 498.38	.2	342
		5, 2, 3← 5, 1, 4		E	0					32 471.40	.2	342
		6, 1, 5← 6, 0, 6		E	0					30 163.59	.2	342
		6, 2, 4← 6, 1, 5		E	0					31 927.71	.2	342
		7, 2, 5← 7, 1, 6		E	0					32 325.08	.2	342
		8, 2, 6← 8, 1, 7		E	0					33 900.78	.2	342

C_3H_5F $C_s(C_{3v},C_s)$ $CH_3CH{:}CHF$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H{:}C^{12}HF^{19}$	C_s	711	42 680. M	3 878.34 M	3 637.02 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
711	1.85 M	0.02 M	0. X		2207	100					

References:

ABC: 189 D_J: D_{JK}: κ: Δ:

μ: 189 eQq: V: 189 I: ω:

Rotational constants (first excited torsional state): B = 3891.52 MHz, C = 3624.22 MHz. Ref. 189.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. State	Rotor n	Hyperfine F_i'	Hyperfine F'	Hyperfine F_i	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H{:}C^{12}HF^{19}$	711	2, 0, 2← 1, 0, 1	Ground	A	0					15 029.68		189
		2, 1, 1← 1, 1, 0	Ground	E	1					15 115.1		189
		2, 1, 1← 1, 1, 0	Ground	E						15 271.35	.1	189
		2, 1, 1← 1, 1, 0	Ground	A	0					15 272.05		189
		2, 1, 1← 1, 1, 0	Ground	A	1					15 298.7		189
		2, 1, 2← 1, 1, 1	Ground	A	1					14 761.		189
		2, 1, 2← 1, 1, 1	Ground	E	0					14 789.20		189
		2, 1, 2← 1, 1, 1	Ground	E						14 789.91	.1	189
		2, 1, 2← 1, 1, 1	Ground	E	1					14 944.2		189
		3, 0, 3← 2, 0, 2	Ground	A	0					22 541.90		189
		3, 1, 2← 2, 1, 1	Ground	E	1					22 784.40		189
		3, 1, 2← 2, 1, 1	Ground	A	0					22 907.60		189
		3, 1, 2← 2, 1, 1	Ground	E						22 908.10	.1	189
		3, 1, 2← 2, 1, 1	Ground	A	1					22 947.90		189
		3, 1, 3← 2, 1, 2	Ground	A	1					22 146.00		189
		3, 1, 3← 2, 1, 2	Ground	A	0					22 183.49		189
		3, 1, 3← 2, 1, 2	Ground	E						22 184.00	.1	189
		3, 1, 3← 2, 1, 2	Ground	E	1					22 308.50		189
		3, 2, 1← 2, 2, 0	Ground	E						22 548.08	.1	189
		3, 2, 1← 2, 2, 0	Ground	A	0					22 550.06		189
		3, 2, 2← 2, 2, 1	Ground	A	0					22 546.07		189
		3, 2, 2← 2, 2, 1	Ground	E						22 548.10	.1	189
		4, 0, 4← 3, 0, 3	Ground	A	0					30 081.20		189
		4, 1, 3← 3, 1, 2	Ground	E	1					30 486.4		189
		4, 1, 3← 3, 1, 2	Ground	A	0					30 542.05		189
		4, 1, 3← 3, 1, 2	Ground	A	1					30 596.0		189
		4, 1, 4← 3, 1, 3	Ground	A	1					29 527.6		189
		4, 1, 4← 3, 1, 3	Ground	A	0					29 576.65		189
		4, 1, 4← 3, 1, 3	Ground	E	1					29 638.0		189
		4, 2, 2← 3, 2, 1	Ground	A	0					30 071.05		189
		4, 2, 2← 3, 2, 1	Ground	E						30 075.50	.1	189
		4, 2, 3← 3, 2, 2	Ground	E						30 056.33	.1	189
		4, 2, 3← 3, 2, 2	Ground	A	0					30 060.63		189
		4, 3, 1← 3, 3, 0	Ground	A	0					30 063.60		189
		4, 3, 2← 3, 3, 1	Ground	A	0					30 063.60		189
		5, 0, 5← 4, 0, 4	Ground	A	0					37 554.80		189
		5, 1, 5← 4, 1, 4	Ground	A	0					36 968.20		189
		5, 2, 3← 4, 2, 2	Ground	E						37 590.00	.1	189
		5, 2, 3← 4, 2, 2	Ground	A	0					37 595.6		189
		5, 3, 2← 4, 3, 1	Ground	A	0					37 580.50		189
		5, 3, 3← 4, 3, 2	Ground	A	0					37 580.50		189

C_3H_5F $C_s(C_{3v},C_s)$ $CH_3CF:CH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}F^{19}:C^{12}H_2$	C_s	721	10 169.40 M	9 041.36 M	4 927.16 M			.56963	3.023

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
721	0.92 M	1.31 M	0. X		2440	16					

References:

ABC: 264 D_J: D_{JK}: κ: 264 Δ: 264

μ: 264 eQq: V: 264 I: ω:

$V_3 = 2432 \pm 11$ cal/mol. Asymmetry Parameter for first exc. state: $\kappa = .565268$. Coupling Parameter: $I_\alpha = 3.11$ amu A^2. Rotational constants for first exc. state: A = 10163.05 MHz, B = 9024.19 MHz., C = 4923.68 MHz. $V_6 < 50$ cal/mol. Ref: 264.

2-Fluoropropene

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}F^{19}:C^{12}H_2$	721	1, 0, 1← 0, 0, 0	Ground	A	1					13 948.05	.1	264
		1, 0, 1← 0, 0, 0	Ground							13 968.65	.1	264
		1, 1, 1← 0, 0, 0	Ground							15 096.93	.1	264
		2, 0, 2← 1, 0, 1	Ground	A	1					24 727.07	.1	264
		2, 0, 2← 1, 0, 1	Ground	E	1					24 728.61	.1	264
		2, 0, 2← 1, 0, 1	Ground							24 749.12	.1	264
		2, 0, 2← 1, 1, 1	Ground	E	1					23 589.01	.1	264
		2, 0, 2← 1, 1, 1	Ground	A	1					23 589.65	.1	264
		2, 0, 2← 1, 1, 1	Ground							23 621.03	.1	264
		2, 1, 2← 1, 0, 1	Ground	A	1					24 932.50	.1	264
		2, 1, 2← 1, 0, 1	Ground	E	1					24 935.22	.1	264
		2, 1, 2← 1, 0, 1	Ground							24 950.96	.1	264
		2, 1, 2← 1, 1, 1	Ground	A	1					23 795.23	.1	264
		2, 1, 2← 1, 1, 1	Ground							23 822.91	.1	264
		2, 1, 1← 2, 0, 2	Ground							12 545.38	.1	264
		2, 1, 1← 2, 1, 2	Ground							12 343.48	.1	264
		2, 2, 1← 2, 1, 2	Ground							15 727.42	.1	264
		3, 1, 2← 3, 0, 3	Ground							22 562.48	.1	264
		3, 2, 1← 3, 1, 2	Ground	A	1					11 724.93	.1	264
		3, 2, 1← 3, 1, 2	Ground	E	1					11 725.89	.1	264
		3, 2, 1← 3, 1, 2	Ground							11 760.50	.1	264
		3, 2, 2← 3, 1, 3	Ground	A	1					23 465.32	.1	264
		3, 2, 2← 3, 1, 3	Ground	E	1					23 472.10	.1	264
		3, 2, 2← 3, 1, 3	Ground							23 509.02	.1	264
		3, 2, 1← 3, 2, 2	Ground							10 790.88	.1	264
		3, 3, 0← 3, 2, 1	Ground							8 892.53	.1	264
		4, 2, 4← 4, 1, 3	Ground							21 481.14	.1	264
		4, 2, 2← 4, 2, 3	Ground							21 323.23	.1	264
		4, 3, 1← 4, 2, 2	Ground	A	1					11 521.81	.1	264
		4, 3, 1← 4, 2, 2	Ground	E	1					11 525.52	.1	264

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}F^{19}$:$C^{12}H_2$	721	4, 3, 1← 4, 2, 2	Ground							11 542.43	.1	264
		4, 3, 2← 4, 2, 3	Ground	A	1					23 975.38	.1	264
		4, 3, 2← 4, 2, 3	Ground	E	1					23 983.98	.1	264
		4, 3, 2← 4, 2, 3	Ground							24 010.42	.1	264
		4, 3, 1← 4, 3, 2	Ground							8 855.45	.1	264
		4, 4, 0← 4, 3, 1	Ground							12 389.35	.1	264
		4, 4, 0← 4, 3, 1	Ground	A	1					12 458.58	.1	264
		4, 4, 0← 4, 3, 1	Ground	E	1					12 483.38	.1	264
		4, 4, 1← 4, 3, 2	Ground							19 977.08	.1	264
		5, 3, 2← 5, 2, 3	Ground							19 977.08	.1	264
		5, 3, 2← 5, 3, 3	Ground							19 369.15	.1	264
		5, 4, 1← 5, 3, 2	Ground							12 291.71	.1	264
		5, 4, 1← 5, 3, 2	Ground	A	1					12 301.64	.1	264
		5, 4, 1← 5, 3, 2	Ground	E	1					12 311.73	.1	264
		5, 4, 2← 5, 3, 3	Ground	A	1					24 924.15	.1	264
		5, 4, 2← 5, 3, 3	Ground	E	1					24 935.22	.1	264
		5, 4, 2← 5, 3, 3	Ground							24 943.63	.1	264
		5, 5, 0← 5, 4, 1	Ground							16 984.60	.1	264
		5, 5, 1← 5, 4, 2	Ground							23 028.32	.1	264
		6, 4, 2← 6, 3, 3	Ground							18 479.63	.1	264
		6, 4, 2← 6, 4, 3	Ground	E	1					16 639.41	.1	264
		6, 4, 2← 6, 4, 3	Ground	A	1					16 651.87	.1	264
		6, 4, 2← 6, 4, 3	Ground							16 778.12	.1	264
		6, 5, 1← 6, 4, 2	Ground							14 285.60	.1	264
		6, 5, 1← 6, 4, 2	Ground	A	1					14 342.40	.1	264
		6, 5, 1← 6, 4, 2	Ground	E	1					14 363.37	.1	264
		7, 5, 2← 7, 5, 3	Ground	E	1					13 589.71	.1	264
		7, 5, 2← 7, 5, 3	Ground	A	1					13 606.97	.1	264
		7, 5, 2← 7, 5, 3	Ground							13 753.18	.1	264
		7, 6, 1← 7, 5, 2	Ground							17 668.70	.1	264
		8, 5, 3← 8, 5, 4	Ground	E	1					26 107.98	.1	264
		8, 5, 3← 8, 5, 4	Ground	A	1					26 125.28	.1	264
		8, 6, 2← 8, 5, 3	Ground	A	1					17 723.34	.1	264
		8, 6, 2← 8, 5, 3	Ground							17 727.50	.1	264
		8, 6, 2← 8, 5, 3	Ground	E	1					17 734.82	.1	264
		8, 6, 2← 8, 6, 3	Ground	E	1					10 379.75	.1	264
		8, 6, 2← 8, 6, 3	Ground	A	1					10 399.20	.1	264
		8, 6, 2← 8, 6, 3	Ground							10 556.52	.1	264
		8, 7, 1← 8, 6, 2	Ground	E	0					22 347.90	.1	264
		8, 7, 1← 8, 6, 2	Ground	A	0					22 348.72	.1	264
		9, 6, 3← 9, 5, 4	Ground	E	1					24 959.57	.1	264
		9, 6, 3← 9, 5, 4	Ground	A	1					24 969.90	.1	264
		9, 6, 3← 9, 5, 4	Ground							25 116.76	.1	264
		9, 6, 3← 9, 6, 4	Ground	A	0					22 866.67	.1	264
		9, 6, 3← 9, 6, 4	Ground	E	0					22 867.00	.1	264
		9, 7, 2← 9, 6, 3	Ground	E	0					19 318.79	.1	264
		9, 7, 2← 9, 6, 3	Ground	A	0					19 319.22	.1	264
		10, 7, 3←10, 6, 4	Ground	E	1					23 411.49	.1	264
		10, 7, 3←10, 6, 4	Ground	A	1					23 415.40	.1	264
		10, 7, 3←10, 6, 4	Ground							23 524.40	.1	264

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. State	Rotor n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}F^{19}:C^{12}H_2$	721	10, 7, 3←10, 7, 4	Ground	A	0					18 900.32	.1	264
		10, 7, 3←10, 7, 4	Ground	E	0					18 900.98	.1	264
		10, 8, 2←10, 7, 3	Ground	E	0					22 496.34	.1	264
		10, 8, 2←10, 7, 3	Ground	A	0					22 497.12	.1	264
		11, 8, 3←11, 7, 4	Ground	A	1					23 039.75	.1	264
		11, 8, 3←11, 7, 4	Ground	E	1					23 048.95	.1	264
		11, 8, 3←11, 7, 4	Ground							23 072.82	.1	264
		11, 8, 3←11, 8, 4	Ground	E	1					14 427.78	.1	264
		11, 8, 3←11, 8, 4	Ground	A	1					14 463.24	.1	264
		11, 8, 3←11, 8, 4	Ground	A	0					14 732.60	.1	264
		11, 8, 3←11, 8, 4	Ground	E	0					14 733.20	.1	264
		12, 9, 3←12, 8, 4	Ground	E	0					24 187.55	.1	264
		12, 9, 3←12, 8, 4	Ground	A	0					24 188.04	.1	264
		12, 9, 3←12, 8, 4	Ground	A	1					24 256.57	.1	264
		12, 9, 3←12, 8, 4	Ground	E	1					24 285.62	.1	264
		12, 9, 3←12, 9, 4	Ground	E	1					10 433.24	.1	264
		12, 9, 3←12, 9, 4	Ground	A	1					10 467.23	.1	264
		12, 9, 3←12, 9, 4	Ground	A	0					10 727.50	.1	264
		12, 9, 3←12, 9, 4	Ground	E	0					10 728.17	.1	264
		13, 9, 4←13, 9, 5	Ground	A	0					24 322.79	.1	264
		13, 9, 4←13, 9, 5	Ground	E	0					24 323.70	.1	264
		14,10, 4←14,10, 5	Ground	A	0					19 253.42	.1	264
		14,10, 4←14,10, 5	Ground	E	0					19 254.38	.1	264
		15,11, 4←15,11, 5	Ground	A	0					14 325.40	.1	264
		15,11, 4←15,11, 5	Ground	E	0					14 326.40	.1	264
		16,12, 4←16,12, 5	Ground	A	0					9 950.12	.1	264
		16,12, 4←16,12, 5	Ground	E	0					9 950.92	.1	264
		17,12, 5←17,12, 6	Ground	A	0					24 117.22	.1	264
		17,12, 5←17,12, 6	Ground	E	0					24 118.48	.1	264
		19,14, 5←19,14, 6	Ground	A	0					13 019.59	.1	264
		19,14, 5←19,14, 6	Ground	E	0					13 020.78	.1	264
		20,15, 5←20,15, 6	Ground	A	0					8 668.27	.1	264
		20,15, 5←20,15, 6	Ground	E	0					8 669.25	.1	264
		21,15, 6←21,15, 7	Ground	A	0					22 635.18	.1	264
		21,15, 6←21,15, 7	Ground	E	0					22 636.78	.1	264
		22,16, 6←22,16, 7	Ground	A	0					16 460.77	.1	264
		22,16, 6←22,16, 7	Ground	E	0					16 462.12	.1	264
		23,17, 6←23,17, 7	Ground	A	0					11 235.41	.1	264
		23,17, 6←23,17, 7	Ground	E	0					11 236.52	.1	264
		25,18, 7←25,18, 8	Ground	A	0					20 278.56	.1	264
		25,18, 7←25,18, 8	Ground	E	0					20 280.18	.1	264
		26,19, 7←26,19, 8	Ground	A	0					14 157.08	.1	264
		26,19, 7←26,19, 8	Ground	E	0					14 158.38	.1	264
		27,20, 7←27,20, 8	Ground	A	0					9 307.38	.1	264
		27,20, 7←27,20, 8	Ground	E	0					9 308.35	.1	264
		28,20, 8←28,20, 9	Ground	A	0					24 475.02	.1	264
		28,20, 8←28,20, 9	Ground	E	0					24 477.02	.1	264
		29,21, 8←29,21, 9	Ground	A	0					17 444.90	.1	264
		29,21, 8←29,21, 9	Ground	E	0					17 446.35	.1	264
		30,22, 8←30,22, 9	Ground	A	0					11 726.82	.1	264
		30,22, 8←30,22, 9	Ground	E	0					11 727.84	.1	264

C_3H_5N $C_s(C_{3v}.C_s)$ C_2H_5CN

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2C^{12}N^{14}$	C_s	731	27 663.30 M	4 714.14 M	4 235.14 M	.0035	−.0496	−.96	
$C^{12}H_3C^{12}H_2C^{13}N^{14}$	C_s	732	27 200. M	4 689.77 M	4 214.87 M				
$C^{12}D_3C^{12}HDC^{12}N^{14}$	C_1	733	20 400. M	4 169.47 M	3 736.83 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
731	3.78 M	1.38 M	0. X	−3.3	3050			220 1			

References:

ABC: 178, 249 D_J: 249 D_{JK}: 249 κ: 249 Δ:

μ: 249 eQq: 249 V: 249 I: ω: 394

Propionitrile

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2C^{12}N^{14}$	731	1, 1, 0← 1, 0, 1	Ground						23 428.1	.2	249
		2, 0, 2← 1, 0, 1	Ground						17 891.0	.2	249
		2, 0, 2← 1, 0, 1	Ground	A 1					17 896.9	.2	249[1]
		2, 0, 2← 1, 0, 1	1						17 920.3	.2	249
		2, 1, 1← 1, 1, 0	Ground						18 377.5	.2	249
		2, 1, 1← 1, 1, 0	1						18 398.0	.2	249
		2, 1, 2← 1, 1, 1	Ground						17 419.8	.2	249
		2, 1, 2← 1, 1, 1	Ground	A 1					17 431.3	.2	249[1]
		2, 1, 2← 1, 1, 1	1						17 457.6	.2	249
		2, 1, 1← 2, 0, 2	Ground						23 915.0	.2	249
		3, 0, 3← 2, 0, 2	Ground						26 817.80	.1	249
		3, 0, 3← 2, 0, 2	Ground	A 1					26 829.3	.2	249[1]
		3, 0, 3← 2, 0, 2	1						26 860.5	.2	249
		3, 1, 2← 2, 1, 1	Ground						27 561.71	.1	249
		3, 1, 2← 2, 1, 1	Ground	A 1					27 562.9	.2	249[1]
		3, 1, 2← 2, 1, 1	Excited						27 576.62	.1	178
		3, 1, 2← 2, 1, 1	1						27 592.2	.2	249
		3, 1, 3← 2, 1, 2	Ground						26 124.57	.1	249
		3, 1, 3← 2, 1, 2	Excited						26 143.64	.1	178
		3, 1, 3← 2, 1, 2	Ground	A 1					26 144.2	.2	249[1]
		3, 1, 3← 2, 1, 2	Excited						26 180.33	.1	178
		3, 1, 3← 2, 1, 2	1						26 180.7	.2	249
		3, 2, 1← 2, 2, 0	Ground			3		2	26 877.45	.1	249
		3, 2, 1← 2, 2, 0	Ground						26 878.27	.1	249
		3, 2, 1← 2, 2, 0	Ground	E 1					26 878.3	.2	249
		3, 2, 1← 2, 2, 0	Ground			4		3	26 878.54	.1	249
		3, 2, 1← 2, 2, 0	Ground			2		1	26 879.08	.1	249
		3, 2, 1← 2, 2, 0	Ground	A 1					26 885.3	.2	249[1]
		3, 2, 1← 2, 2, 0	1						26 922.1	.2	249
		3, 2, 2← 2, 2, 1	Ground			3		2	26 847.89	.1	249

1 See footnote at end of table.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2C^{12}N^{14}$	731	3, 2, 2← 2, 2, 1	Ground							26 848.70	.1	249
		3, 2, 2← 2, 2, 1	Ground				4		3	26 848.95	.1	249
		3, 2, 2← 2, 2, 1	Ground				2		1	26 849.51	.1	249
		3, 2, 2← 2, 2, 1	Ground	A	1					26 859.1	.2	249[1]
		3, 2, 2← 2, 2, 1	Ground	E	1					26 866.1	.2	249
		3, 2, 2← 2, 2, 1	1							26 889.6	.2	249
		3, 1, 2← 3, 0, 3	Ground							24 658.69	.1	249
		4, 0, 4← 3, 0, 3	Ground							35 722.18	.1	249
		4, 0, 4← 3, 0, 3	Ground	A	1					35 742.5	.2	249[1]
		4, 0, 4← 3, 0, 3	1							35 776.5	.2	249
		4, 1, 4← 3, 1, 3	Ground							34 824.10	.1	249
		4, 1, 4← 3, 1, 3	1							34 898.0	.2	249
		4, 1, 4← 3, 1, 3	Ground	A	1					35 855.2	.2	249[1]
		4, 2, 2← 3, 2, 1	Ground							35 866.1	.2	249
		4, 2, 2← 3, 2, 1	Ground	E	1					35 867.6	.2	249
		4, 2, 2← 3, 2, 1	Ground	A	1					35 871.8	.2	249[1]
		4, 2, 2← 3, 2, 1	1							35 926.0	.2	249
		4, 2, 3← 3, 2, 2	Ground				4		3	35 791.80	.1	249
		4, 2, 3← 3, 2, 2	Ground							35 792.1	.2	249
		4, 2, 3← 3, 2, 2	Ground				5		4	35 792.29	.1	249
		4, 2, 3← 3, 2, 2	Ground				3		2	35 792.29	.1	249
		4, 2, 3← 3, 2, 2	Ground	A	1					35 806.3	.2	249[1]
		4, 2, 3← 3, 2, 2	Ground	E	1					35 810.8	.2	249
		4, 2, 3← 3, 2, 2	1							35 844.6	.2	249
		4, 3, 1← 3, 3, 0	Ground				4		3	35 813.85	.1	249
		4, 3, 1← 3, 3, 0	Ground							35 814.6	.2	249
		4, 3, 1← 3, 3, 0	Ground				5		4	35 814.96	.1	249
		4, 3, 1← 3, 3, 0	Ground				3		2	35 814.96	.1	249
		4, 3, 1← 3, 3, 0	Ground	A	1					35 830.4	.2	249[1]
		4, 3, 1← 3, 3, 0	1							35 861.4	.2	249
		4, 3, 2← 3, 3, 1	Ground				4		3	35 813.85	.1	249
		4, 3, 2← 3, 3, 1	Ground							35 814.6	.2	249
		4, 3, 2← 3, 3, 1	Ground				5		4	35 814.96	.1	249
		4, 3, 2← 3, 3, 1	Ground				3		2	35 814.96	.1	249
		4, 3, 2← 3, 3, 1	Ground	A	1					35 830.4	.2	249[1]
		4, 3, 2← 3, 3, 1	1							35 861.4	.2	249
		4, 1, 3← 4, 0, 4	Ground							25 676.20	.1	249
		5, 0, 5← 4, 1, 4	Ground							23 710.80	.1	249
		5, 1, 4← 5, 0, 5	Ground							26 988.70	.1	249
		6, 1, 5← 6, 0, 6	Ground							28 622.28	.1	249
		Not Reported	Excited							27 626.49	.1	178
$C^{12}H_3C^{12}H_2C^{13}N^{14}$	732	3, 0, 3← 2, 0, 2	Ground							26 684.09	.1	178
		3, 1, 2← 2, 1, 1	Ground							27 421.62	.1	178
		3, 1, 3← 2, 1, 2	Ground							25 996.90	.1	178
		3, 2, 1← 2, 2, 0	Ground							26 743.8	.5	178
		3, 2, 2← 2, 2, 1	Ground							26 713.9	.5	178
$C^{12}D_3C^{12}HDC^{12}N^{14}$	733	3, 0, 3← 2, 0, 2	Ground							23 684.68	.1	178
		3, 1, 2← 2, 1, 1	Ground							24 362.51	.1	178
		3, 1, 3← 2, 1, 2	Ground							23 064.59	.1	178
		3, 2, 1← 2, 2, 0	Ground							23 745.08	.1	178
		3, 2, 2← 2, 2, 1	Ground							23 719.06	.1	178

1. The lines in the first excited torsional state identified to be of the A species may be of the unresolved AE states.

C_3H_6 $C_s(C_{3v},C_1,C_{2v})$ $CH_3CH{:}CH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H{:}C^{12}H_2$	C_s	741	46 070. M	9 305.28 M	8 134.16 M				105.5
a-$C^{12}H_2DC^{12}H{:}C^{12}H_2$	C_1	742	44 085. M	8 658.80 M	7 718.14 M				
s-$C^{12}H_2DC^{12}H{:}C^{12}H_2$	C_s	743	40 615. M	9 066.92 M	7 765.90 M				
$C^{12}H_3C^{13}H{:}C^{12}H_2$	C_s	744	45 296. M	9 304.16 M	8 107.13 M				101.6
c-$C^{12}H_3C^{12}H{:}C^{12}HD$	C_1	745	M	9 037.30 M	7 727.27 M				
t-$C^{12}H_3C^{12}H{:}C^{12}HD$	C_1	746	M	8 545.34 M	7 539.87 M				
$C^{12}H_3C^{12}D{:}C^{12}H_2$	C_s	747	M	9 298.96 M	7 834.74 M				
$C^{13}H_3C^{12}H{:}C^{12}H_2$	C_s	748	M	9 045.15 M	7 930.54 M				
$C^{12}H_3C^{12}H{:}C^{13}H_2$	C_s	749	M	9 045.54 M	7 928.40 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
741	0.360 M	0.05 M	0. X		1978	17					

References:

ABC: 181, 213, 327 D_J: D_{JK}: κ: Δ: 181

μ: 181 eQq: V: 181 I: ω:

Add. Ref.: 298

Coupling Parameter: $I_\alpha = 3.120$ amu Å^2. Ref: 326.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H{:}C^{12}H_2$	741	1, 0, 1← 0, 0, 0	Ground							17 439.49	.03	181
		2, 0, 2← 1, 0, 1	Ground	E	0					34 851.27	.03	181
		2, 0, 2← 1, 0, 1	Ground	A	0					34 851.52	.03	181
		2, 1, 1← 1, 1, 0	Ground	E	0					36 049.29	.03	181
		2, 1, 1← 1, 1, 0	Ground	A	0					36 050.21	.03	181
		2, 1, 2← 1, 1, 1	Ground	A	0					33 707.81	.03	181
		2, 1, 2← 1, 1, 1	Ground	E	0					33 708.26	.03	181
a-$C^{12}H_2DC^{12}H{:}C^{12}H_2$	742	1, 0, 1← 0, 0, 0	Ground							16 377.15	.15	213
		2, 0, 2← 1, 0, 1	Ground							32 735.34	.05	327
		2, 1, 1← 1, 1, 0	Ground							33 695.17	.05	327
		2, 1, 2← 1, 1, 1	Ground							31 813.36	.05	327
s-$C^{12}H_2DC^{12}H{:}C^{12}H_2$	743	1, 0, 1← 0, 0, 0	Ground							16 832.90	.15	213
		2, 0, 2← 1, 0, 1	Ground							33 626.41	.05	327
		2, 1, 1← 1, 1, 0	Ground							34 966.94	.05	327
		2, 1, 2← 1, 1, 1	Ground							32 364.93	.05	327
$C^{12}H_3C^{13}H{:}C^{12}H_2$	744	1, 0, 1← 0, 0, 0	Ground							17 411.29	.03	181
		2, 0, 2← 1, 0, 1	Ground	E	0					34 793.13	.03	181
		2, 0, 2← 1, 0, 1	Ground	A	0					34 793.38	.03	181
		2, 1, 1← 1, 1, 0	Ground	E	0					36 019.03	.03	181
		2, 1, 1← 1, 1, 0	Ground	A	0					36 019.84	.03	181
		2, 1, 2← 1, 1, 1	Ground	A	0					33 625.62	.03	181
		2, 1, 2← 1, 1, 1	Ground	E	0					33 626.01	.03	181
c-$C^{12}H_3C^{12}H{:}C^{12}HD$	745	2, 0, 2← 1, 0, 1	Ground							33 499.06	.05	327
		2, 1, 1← 1, 1, 0	Ground	E	0					34 849.69	.05	327
		2, 1, 1← 1, 1, 0	Ground							34 850.14	.05	327
		2, 1, 2← 1, 1, 1	Ground							32 229.17	.05	327
t-$C^{12}H_3C^{12}H{:}C^{12}HD$	746	2, 0, 2← 1, 0, 1	Ground	A	0					32 160.37	.05	327
		2, 1, 1← 1, 1, 0	Ground	E	0					31 185.46	.05	327
		2, 1, 1← 1, 1, 0	Ground	A	0					33 186.35	.05	327
		2, 1, 2← 1, 1, 1	Ground	A	0					31 174.64	.05	327
		2, 1, 2← 1, 1, 1	Ground	E	0					31 175.18	.05	327
$C^{12}H_3C^{12}D{:}C^{12}H_2$	747	2, 0, 2← 1, 0, 1	Ground							34 223.64	.05	327
		2, 1, 1← 1, 1, 0	Ground	E	0					35 742.37	.05	327
		2, 1, 1← 1, 1, 0	Ground							35 742.81	.05	327
		2, 1, 2← 1, 1, 1	Ground							32 813.39	.05	327
$C^{13}H_3C^{12}H{:}C^{12}H_2$	748	2, 0, 2← 1, 0, 1	Ground							33 937.14	.10	327
		2, 1, 1← 1, 1, 0	Ground	E	0					35 076.09	.7	327
		2, 1, 1← 1, 1, 0	Ground							35 077.02	.10	327
		2, 1, 2← 1, 1, 1	Ground							32 847.20	.10	327
$C^{12}H_3C^{12}H{:}C^{13}H_2$	749	2, 0, 2← 1, 0, 1	Ground							33 933.42	.10	327
		2, 1, 1← 1, 1, 0	Ground	E	0					35 075.07	.7	327
		2, 1, 1← 1, 1, 0	Ground							35 076.09	.10	327
		2, 1, 2← 1, 1, 1	Ground							32 841.16	.10	327

C_3H_6O $C_{2v}(C_{3v},C_{3v},C_{2v})$ $(CH_3)_2CO$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_2C^{12}O^{16}$	C_{2v}	751	10 165.20 M	8 515.27 M	4 910.15 M				
$(C^{12}D_3)_2C^{12}O^{16}$	C_{2v}	752	8 469.40 M	6 419.60 M	4 011.28 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
751	0. X	2.90 M	0. X		274						
752					258						

References:

ABC: 271 D_J: D_{JK}: κ: Δ:

μ: 271 eQq: V: 271 I: ω:

Add. Refs.: 62, 237

Rotational Constants:

$(C^{12}H_3)_2C^{12}O^{16}$	Torsional State	$(C^{12}D_3)_2C^{12}O^{16}$
A = 10185.99 MHz B = 8519.75 MHz C = 4910.05 MHz	A and B	A = 8471.50 MHz B = 6420.00 MHz C = 4011.26 MHz
A = 10170.40 MHz B = 8516.33 MHz C = 4910.15 MHz	Q	A = 8469.94 MHz B = 6419.68 MHz C = 4011.28 MHz
A = 10154.81 MHz B = 8513.10 MHz C = 4910.15 MHz	E	A = 8468.34 MHz B = 6419.42 MHz C = 4011.30 MHz
I_α = 3.138	Rotational Parameter Ref: 271.	I_α = 6.272

Acetone

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2C^{12}O^{16}$	751	1, 1, 1← 0, 0, 0	Ground	EE	0					15 038.47	.04	271[2]
		1, 1, 1← 0, 0, 0	Ground	E_3	0					15 064.91	.04	271
		1, 1, 1← 0, 0, 0	Ground	EE	0					15 074.05	.04	271[1]
		1, 1, 1← 0, 0, 0	Ground	A	0					15 096.36	.04	271
		2, 0, 2← 1, 1, 1	Ground	EE	0					20 820.89	.04	271[2]
		2, 0, 2← 1, 1, 1	Ground		0					22 793.22	.04	271
		2, 0, 2← 1, 1, 1	Ground	E_3	0					22 794.24	.04	271
		2, 0, 2← 1, 1, 1	Ground	EE	0					22 800.37	.04	271[1]
		2, 1, 2← 1, 0, 1	Ground	EE	0					24 876.48	.04	271[2]
		2, 1, 2← 1, 0, 1	Ground	E_3	0					24 888.30	.04	271
		2, 1, 2← 1, 0, 1	Ground	EE	0					24 899.44	.04	271[1]
		2, 1, 2← 1, 0, 1	Ground	A	0					24 916.41	.04	271
		2, 2, 1← 1, 1, 0	Ground	EE	0					35 220.0	.04	271[2]
		2, 2, 1← 1, 1, 0	Ground	E_3	0					35 371.46	.04	271
		2, 2, 1← 1, 1, 0	Ground	EE	0					35 381.40	.04	271[1]

1. These lines correspond to the Q levels in Swalen and Costain's article. Due to incompatibility of notation they were indicated only as doubly-degenerate excited lines.

2. These lines correspond to the E_1 and E_2 lines in Swalen and Costain's article. Due to incompatibility of notation they were indicated only as doubly-degenerate excited lines.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2C^{12}O^{16}$	751	2, 2, 1← 1, 1, 0	Ground	A	0					35 468.06	.04	271
		Not Reported								22 410.	5.	19
		Not Reported								22 500.	5.	19
		Not Reported								22 560.	5.	19
		Not Reported								22 940.	5.	19
		Not Reported								23 339.	5.	19
		Not Reported								23 603.	5.	19
		Not Reported								23 661.	5.	19
		Not Reported								23 749.	5.	19
		Not Reported								23 778.	5.	19
		Not Reported								23 793.	5.	19
		Not Reported								23 827.	5.	19
		Not Reported								23 839.	5.	19
		Not Reported								23 934.	5.	19
		Not Reported								24 102.	5.	19
		Not Reported								24 646.	5.	19
		Not Reported								24 691.	5.	19
		Not Reported								24 758.	5.	19
		Not Reported								26 661.5		62
		Not Reported								28 340.0		62
		Not Reported								28 622.3		62
		Not Reported								30 070.		62
$(C^{12}D_3)_2C^{12}O^{16}$	752	1, 1, 1← 0, 0, 0	Ground	E	0					12 479.45	.04	271
		1, 1, 1← 0, 0, 0	Ground	EE	0					12 481.21	.04	271[1]
		1, 1, 1← 0, 0, 0	Ground	A	0					12 482.76	.04	271
		2, 0, 2← 1, 1, 1	Ground	A	0					17 589.27	.04	271
		2, 0, 2← 1, 1, 1	Ground	EE	0					17 589.80	.04	271[1]
		2, 0, 2← 1, 1, 1	Ground	E	0					17 590.35	.04	271
		2, 1, 2← 1, 0, 1	Ground	E	0					20 502.24	.04	271
		2, 1, 2← 1, 0, 1	Ground	EE	0					20 503.80	.04	271[1]
		2, 1, 2← 1, 0, 1	Ground	A	0					20 505.26	.04	271
		2, 2, 0← 1, 1, 1	Ground	E_3	0					33 046.62	.04	271
		2, 2, 0← 1, 1, 1	Ground	E_1	0					33 047.70	.04	271
		2, 2, 0← 1, 1, 1	Ground	EE	0					33 051.65	.04	271[1]
		2, 2, 0← 1, 1, 1	Ground	A	0					33 056.22	.04	271
		2, 2, 1← 1, 1, 0	Ground	E_2	0					29 415.18	.04	271
		2, 2, 1← 1, 1, 0	Ground	E_3	0					29 416.28	.04	271
		2, 2, 1← 1, 1, 0	Ground	EE	0					29 420.63	.04	271[1]
		2, 2, 1← 1, 1, 0	Ground	A	0					29 425.84	.04	271
		3, 2, 2← 2, 1, 1	Ground	E	0					37 438.80	.04	271
		3, 2, 2← 2, 1, 1	Ground	EE	0					37 443.15	.04	271[1]
		3, 2, 2← 2, 2, 1	Ground	A	0					37 447.95	.04	271

1. These lines correspond to the Q levels in Swalen and Costain's article. Due to incompatibility of notation they were indicated only as doubly-degenerate excited lines.

760 - 1,2-Epoxypropane

Propylene Oxide; Propene Oxide; Methyloxirane

Molecular Constant Table

C_3H_6O $C_1(C_{3v},C_1)$ $CH_3C^*HOC^*H_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	C_1	761	18 023.72 M	6 682.12 M	5 951.48 M	2.97	4.20	−.8790	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
761	0.95 M	1.67 M	0.56 M		2560	70					

References:

ABC: 191 D_J: 212 D_{JK}: 212 κ: 191 Δ:

μ: 191 eQq: V: 212 I: ω:

Coupling parameter: $I_\alpha = 3.194$ amu Å^2. $\Delta_0 = 4.11$ MHz. Ref: 212.
Rotational constants (v = 1): for state A, A = 18010.82 MHz, B = 6669.93 MHz, and C = 5944.82 MHz; for state E, A = 18016.20 MHz, B = 6670.01 MHz, and C = 5945.10 MHz. Asymmetry parameters (v = 1): for state A, $\kappa = -.879809$; for state E, $\kappa = -.879893$. Ref: 191.

1,2-Epoxypropane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	1, 0, 1← 0, 0, 0	Ground	E	2					12 595.01	.1	214
		1, 0, 1← 0, 0, 0	Ground	A	2					12 598.99	.1	214
		1, 0, 1← 0, 0, 0	Ground		1					12 614.92	.1	214
		1, 0, 1← 0, 0, 0	Ground							12 633.52	.1	214
		1, 1, 0← 0, 0, 0	Ground							24 705.86	.1	214
		1, 1, 1← 0, 0, 0	Ground	A	1					23 955.64	.1	214
		1, 1, 1← 0, 0, 0	Ground	E	1					23 960.29	.1	214
		1, 1, 1← 0, 0, 0	Ground							23 975.20	.1	214
		1, 1, 1← 0, 0, 0	Ground	A	2					24 032.19	.1	214
		1, 1, 0← 1, 0, 1	Ground							12 072.04	.1	214
		1, 1, 1← 1, 0, 1	Ground							11 341.70	.1	214
		2, 0, 2← 1, 0, 1	Ground	E	2					25 156.18	.1	214
		2, 0, 2← 1, 0, 1	Ground	A	2					25 165.43	.1	214
		2, 0, 2← 1, 0, 1	Ground							25 196.48	.1	214
		2, 0, 2← 1, 0, 1	Ground							25 232.90	.1	214
		2, 0, 2← 1, 1, 1	Ground	E	1					13 851.47	.1	214
		2, 0, 2← 1, 1, 1	Ground	A	1					13 855.30	.1	214
		2, 0, 2← 1, 1, 1	Ground							13 891.15	.1	214
		2, 1, 1← 1, 0, 1	Ground	A	1					38 021.11	.1	214
		2, 1, 1← 1, 0, 1	Ground	E	1					38 026.70	.1	214
		2, 1, 1← 1, 0, 1	Ground							38 070.06	.1	214
		2, 1, 2← 1, 0, 1	Ground	E	2					35 566.15	.1	214
		2, 1, 2← 1, 0, 1	Ground	A	1					35 845.46	.1	214
		2, 1, 2← 1, 0, 1	Ground	E	1					35 850.67	.1	214
		2, 1, 2← 1, 0, 1	Ground							35 878.14	.1	214

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	2, 1, 2← 1, 0, 1	Ground	A	2					35 913.04	.1	214
		2, 1, 1← 1, 1, 0	Ground							25 997.85	.1	214
		2, 1, 2← 1, 1, 1	Ground							24 536.55	.1	214
		2, 1, 1← 2, 0, 2	Ground	A	1					12 825.07	.1	214
		2, 1, 1← 2, 0, 2	Ground	E	1					12 830.22	.1	214
		2, 1, 1← 2, 0, 2	Ground							12 837.32	.1	214
		2, 1, 1← 2, 0, 2	Ground	A	2					12 901.27	.1	214
		2, 2, 0← 2, 1, 1	Ground	A	1					34 055.65	.1	214
		2, 2, 0← 2, 1, 1	Ground							34 058.49	.1	214
		2, 2, 0← 2, 1, 1	Ground	E	1					34 111.51	.1	214
		2, 2, 1← 2, 1, 1	Ground	E	1					33 997.63	.1	214
		2, 2, 1← 2, 1, 1	Ground	A	1					34 022.78	.1	214
		2, 2, 1← 2, 1, 1	Ground							34 024.55	.1	214
		2, 2, 1← 2, 1, 2	Ground	E	1					36 173.03	.1	214
		2, 2, 1← 2, 1, 2	Ground	A	1					36 198.17	.1	214
		2, 2, 1← 2, 1, 2	Ground							36 216.40	.1	214
		3, 0, 3← 2, 0, 2	Ground	E	2					37 651.04	.1	214
		3, 0, 3← 2, 0, 2	Ground	A	2					37 666.36	.1	214
		3, 0, 3← 2, 0, 2	Ground							37 710.31	.1	214
		3, 0, 3← 2, 0, 2	Ground							37 764.55	.1	214
		3, 0, 3← 2, 1, 2	Ground	A	2					26 918.07	.1	214
		3, 0, 3← 2, 1, 2	Ground	E	1					27 056.70	.1	214
		3, 0, 3← 2, 1, 2	Ground	A	1					27 061.01	.1	214
		3, 0, 3← 2, 1, 2	Ground							27 119.10	.1	214
		3, 0, 3← 2, 1, 2	Ground	E	2					27 240.85	.1	214
		3, 1, 2← 2, 1, 1	Ground	E	2					38 757.75	.1	214
		3, 1, 2← 2, 1, 1	Ground	A	2					38 852.54	.1	214
		3, 1, 2← 2, 1, 1	Ground		1					38 910.96	.1	214
		3, 1, 2← 2, 1, 1	Ground							38 974.35	.1	214
		3, 1, 3← 2, 1, 2	Ground	A	2					36 700.24	.1	214
		3, 1, 3← 2, 1, 2	Ground	A	1					36 736.13	.1	214
		3, 1, 3← 2, 1, 2	Ground	E	1					36 737.03	.1	214
		3, 1, 3← 2, 1, 2	Ground	E	2					36 774.08	.1	214
		3, 1, 3← 2, 1, 2	Ground							36 783.14	.1	214
		3, 2, 1← 2, 2, 0	Ground	E	2					37 855.93	.1	214
		3, 2, 1← 2, 2, 0	Ground	A	2					37 926.73	.1	214
		3, 2, 1← 2, 2, 0	Ground	E	1					37 954.79	.1	214
		3, 2, 1← 2, 2, 0	Ground	A	1					37 979.00	.1	214
		3, 2, 1← 2, 2, 0	Ground							38 036.22	.1	214
		3, 2, 2← 2, 2, 1	Ground	A	2					37 796.16	.1	214
		3, 2, 2← 2, 2, 1	Ground	A	1					37 844.07	.1	214
		3, 2, 2← 2, 2, 1	Ground	E	2					37 853.03	.1	214
		3, 2, 2← 2, 2, 1	Ground	E	1					37 869.28	.1	214
		3, 2, 2← 2, 2, 1	Ground							37 900.09	.1	214
		3, 1, 2← 3, 0, 3	Ground	A	1					14 025.86	.1	214
		3, 1, 2← 3, 0, 3	Ground	E	1					14 030.68	.1	214
		3, 1, 2← 3, 0, 3	Ground							14 047.52	.1	214
		3, 1, 2← 3, 0, 3	Ground	E	2					14 084.31	.1	214
		3, 1, 2← 3, 0, 3	Ground	A	2					14 087.32	.1	214
		3, 2, 1← 3, 1, 2	Ground							33 120.72	.1	214

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	3, 2, 1← 3, 1, 2	Ground	A	1					33 124.24	.1	214
		3, 2, 1← 3, 1, 2	Ground	E	1					33 155.45	.1	214
		3, 2, 2← 3, 1, 2	Ground							32 950.24	.1	214
		3, 2, 2← 3, 1, 2	Ground		1					32 956.15	.1	214
		3, 2, 2← 3, 1, 3	Ground	E	1					37 305.41	.1	214
		3, 2, 2← 3, 1, 3	Ground	A	1					37 306.66	.1	214
		3, 2, 2← 3, 1, 3	Ground							37 333.28	.1	214
		4, 1, 3← 3, 2, 2	Ground	A	0					18 972.75	.1	214
		4, 1, 3← 3, 2, 2	Ground	E	0					18 973.03	.1	214
		4, 1, 4← 3, 2, 1	Ground							11 502.18	.1	214
		4, 1, 3← 4, 0, 4	Ground	A	1					15 738.20	.1	214
		4, 1, 3← 4, 0, 4	Ground	E	2					15 741.10	.1	214
		4, 1, 3← 4, 0, 4	Ground	E	1					15 742.20	.1	214
		4, 1, 3← 4, 0, 4	Ground							15 775.13	.1	214
		4, 1, 3← 4, 0, 4	Ground	A	2					15 777.87	.1	214
		4, 2, 2← 4, 1, 3	Ground							32 041.80	.1	214
		4, 2, 2← 4, 1, 3	Ground	A	1					32 049.35	.1	214
		4, 2, 2← 4, 1, 3	Ground	E	1					32 065.55	.1	214
		4, 2, 3← 4, 1, 4	Ground							38 834.10	.1	214
		5, 1, 4← 5, 0, 5	Ground	E	2					18 015.71	.1	214
		5, 1, 4← 5, 0, 5	Ground	A	1					18 045.84	.1	214
		5, 1, 4← 5, 0, 5	Ground	E	1					18 048.95	.1	214
		5, 1, 4← 5, 0, 5	Ground	A	2					18 053.85	.1	214
		5, 1, 4← 5, 0, 5	Ground							18 104.06	.1	214
		5, 2, 3← 5, 1, 4	Ground	E	0					30 961.14	.1	214
		5, 2, 3← 5, 1, 4	Ground	A	0					30 961.40	.1	214
		5, 2, 3← 5, 1, 4	Ground	A	1					30 973.40	.1	214
		5, 2, 3← 5, 1, 4	Ground	E	1					30 990.50	.1	214
		6, 2, 4← 5, 3, 3	Ground	A	0					19 105.40	.1	214
		6, 2, 4← 5, 3, 3	Ground	E	0					19 106.02	.1	214
		6, 2, 5← 5, 3, 2	Ground	A	0					16 786.62	.1	214
		6, 2, 5← 5, 3, 2	Ground	E	0					16 786.96	.1	214
		6, 1, 5← 6, 0, 6	Ground	E	2					20 963.10	.1	214
		6, 1, 5← 6, 0, 6	Ground	A	2					20 995.83	.1	214
		6, 1, 5← 6, 0, 6	Ground	A	1					21 029.92	.1	214
		6, 1, 5← 6, 0, 6	Ground	E	1					21 032.25	.1	214
		6, 1, 5← 6, 0, 6	Ground							21 115.40	.1	214
		6, 2, 4← 6, 1, 5	Ground	E	0					30 038.11	.1	214
		6, 2, 4← 6, 1, 5	Ground	A	0					30 038.37	.1	214
		6, 2, 4← 6, 1, 5	Ground	A	1					30 048.77	.1	214
		6, 2, 4← 6, 1, 5	Ground	E	1					30 064.48	.1	214
		6, 5, 2← 7, 4, 3	Ground							16 653.80	.1	214
		7, 2, 5← 6, 3, 4	Ground	A	0					33 018.10	.1	214
		7, 2, 5← 6, 3, 4	Ground	E	0					33 018.62	.1	214
		7, 2, 6← 6, 3, 3	Ground							28 938.18	.1	214
		7, 1, 6← 7, 0, 7	Ground	E	2					24 653.60	.1	214
		7, 1, 6← 7, 0, 7	Ground	A	2					24 663.52	.1	214
		7, 1, 6← 7, 0, 7	Ground	A	1					24 749.23	.1	214
		7, 1, 6← 7, 0, 7	Ground	E	1					24 750.32	.1	214
		7, 1, 6← 7, 0, 7	Ground							24 869.10	.1	214

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	7, 1, 5← 7, 1, 6	Ground							25 436.20	.1	214
		7, 2, 5← 7, 1, 6	Ground	E	0					29 435.25	.1	214
		7, 2, 5← 7, 1, 6	Ground	A	0					29 435.50	.1	214
		7, 2, 5← 7, 1, 6	Ground	A	1					29 438.42	.1	214
		7, 2, 5← 7, 1, 6	Ground	E	1					29 452.50	.1	214
		7, 6, ← 8, 5,	Ground	E	0					27 428.17	.1	214[1]
		7, 6, ← 8, 5,	Ground	E	0					27 428.52	.1	214[1]
		7, 6, ← 8, 5,	Ground	A	0					27 429.04	.1	214[1]
		8, 3, 5← 7, 4, 4	Ground	E	0					20 049.26	.1	214
		8, 3, 5← 7, 4, 4	Ground	A	0					20 053.31	.1	214
		8, 3, 5← 7, 4, 4	Ground	E	0					20 054.58	.1	214
		8, 3, 6← 7, 4, 3	Ground							19 598.51	.1	214
		8, 3, 6← 7, 4, 3	Ground	E	0					19 603.72	.1	214
		8, 1, 7← 8, 0, 8	Ground	A	2					29 075.76	.1	214
		8, 1, 7← 8, 0, 8	Ground	E	2					29 082.36	.1	214
		8, 1, 7← 8, 0, 8	Ground							29 220.78	.1	214
		8, 1, 7← 8, 0, 8	Ground							29 380.35	.1	214
		8, 1, 7← 8, 1, 8	Ground							25 853.9	.1	214
		8, 2, 6← 8, 1, 7	Ground	A	1					29 289.95	.1	214
		8, 2, 6← 8, 1, 7	Ground	E	0					29 301.61	.1	214
		8, 2, 6← 8, 1, 7	Ground	A	0					29 301.82	.1	214
		8, 2, 6← 8, 1, 7	Ground	E	1					29 302.49	.1	214
		8, 2, 7← 8, 1, 7	Ground							22 912.6	.1	214
		8, 6, 3← 9, 5, 4	Ground							14 701.45	.1	214
		9, 3, 6← 8, 4, 5	Ground	A	0					33 247.86	.1	214
		9, 3, 6← 8, 4, 5	Ground	E	0					33 248.84	.1	214
		9, 3, 7← 8, 4, 4	Ground	A	0					32 347.36	.1	214
		9, 3, 7← 8, 4, 4	Ground	E	0					32 347.71	.1	214
		9, 4, 5← 8, 5, 4	Ground	A	0					8 906.22	.1	214
		9, 4, 5← 8, 5, 4	Ground	E	0					8 907.53	.1	214
		9, 1, 8← 9, 0, 9	Ground	A	2					34 201.56	.1	214
		9, 1, 8← 9, 0, 9	Ground	E	2					34 254.08	.1	214
		9, 1, 8← 9, 0, 9	Ground	E	1					34 407.03	.1	214
		9, 1, 8← 9, 0, 9	Ground	A	1					34 408.24	.1	214
		9, 1, 8← 9, 0, 9	Ground							34 611.20	.1	214
		9, 2, 7← 9, 1, 8	Ground	A	1					29 730.32	.1	214
		9, 2, 7← 9, 1, 8	Ground	E	1					29 740.80	.1	214
		9, 2, 7← 9, 1, 8	Ground	E	0					29 764.80	.1	214
		9, 2, 7← 9, 1, 8	Ground	A	0					29 765.05	.1	214
		9, 2, 8← 9, 1, 8	Ground							20 234.15	.1	214
		9, 7, ←10, 6,	Ground	E	0					25 479.05	.1	214[1]
		9, 7, ←10, 6,	Ground	A	0					25 480.04	.1	214[1]
		10, 4, 6← 9, 5, 5	Ground	E	0					21 772.39	.1	214
		10, 4, 6← 9, 5, 5	Ground	A	0					21 774.11	.1	214
		10, 4, 6← 9, 5, 5	Ground	E	0					21 776.73	.1	214
		10, 4, 7← 9, 5, 4	Ground	E	0					21 700.53	.1	214
		10, 4, 7← 9, 5, 4	Ground	A	0					21 701.65	.1	214
		10, 4, 7← 9, 5, 4	Ground	E	0					21 704.80	.1	214
		10, 1, 9←10, 0,10	Ground							40 469.72	.1	214
		10, 2, 8←10, 1, 9	Ground	A	1					30 864.26	.1	214

1. In the labeling of transitions, the K_{+1} subscript has been omitted whenever the asymmetry splitting of the rotational levels is less than .1 MHz.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	10, 2, 8←10, 1, 9	Ground	E	1					30 872.70	.1	214
		10, 2, 8←10, 1, 9	Ground							30 930.46	.1	214
		11, 4, 7←10, 5, 6	Ground	E	0					34 722.35	.1	214
		11, 4, 7←10, 5, 6	Ground	A	0					34 724.83	.1	214
		11, 4, 7←10, 5, 6	Ground	E	0					34 726.82	.1	214
		11, 4, 8←10, 5, 5	Ground	E	0					34 570.45	.1	214
		11, 4, 8←10, 5, 5	Ground	A	0					34 571.04	.1	214
		11, 4, 8←10, 5, 5	Ground	E	0					34 574.92	.1	214
		11, 5, 6←10, 6, 5	Ground	A	0					10 845.88	.1	214
		11, 5, 6←10, 6, 5	Ground	E	0					10 846.38	.1	214
		11, 2, 9←11, 1,10	Ground	A	1					32 777.28	.1	214
		11, 2, 9←11, 1,10	Ground	E	1					32 782.77	.1	214
		11, 2, 9←11, 1,10	Ground							32 883.48	.1	214
		11, 8, ←12, 7,	Ground	E	0					23 526.15	.1	214[1]
		11, 8, ←12, 7,	Ground	A	0					23 527.00	.1	214[1]
		12, 5, 7←11, 6, 6	Ground	E	0					23 679.29	.1	214
		12, 5, 7←11, 6, 6	Ground	A	0					23 680.51	.1	214
		12, 5, 7←11, 6, 6	Ground	E	0					23 683.96	.1	214
		12, 5, 8←11, 6, 5	Ground	E	0					23 668.22	.1	214
		12, 5, 8←11, 6, 5	Ground	A	0					23 670.17	.1	214
		12, 5, 8←11, 6, 5	Ground	E	0					23 672.94	.1	214
		12, 2,10←12, 1,11	Ground		1					35 537.88	.1	214
		12, 2,10←12, 1,11	Ground							35 690.23	.1	214
		13, 5, 8←12, 6, 7	Ground	E	0					36 563.90	.1	214
		13, 5, 8←12, 6, 7	Ground	A	0					36 565.29	.1	214
		13, 5, 8←12, 6, 7	Ground	E	0					36 568.41	.1	214
		13, 5, 9←12, 6, 6	Ground	E	0					36 540.92	.1	214
		13, 5, 9←12, 6, 6	Ground	A	0					36 542.27	.1	214
		13, 5, 9←12, 6, 6	Ground	E	0					36 545.43	.1	214
		13, 6, 7←12, 7, 6	Ground	A	0					12 801.74	.1	214
		13, 6, 7←12, 7, 6	Ground	E	0					12 802.48	.1	214
		13, 2,11←13, 1,12	Ground							39 388.43	.1	214
		13, 9, ←14, 8,	Ground	E	0					21 568.32	.1	214[1]
		13, 9, ←14, 8,	Ground	A	0					21 569.20	.1	214[1]
		14, 6, 8←13, 7, 7	Ground							25 623.46	.1	214
		14, 6, 9←13, 7, 6	Ground	A	0					25 622.24	.1	214
		14, 6, 9←13, 7, 6	Ground	E	0					25 623.66	.1	214
		15, 7, ←14, 8,	Ground	A	0					14 760.68	.1	214[1]
		15, 7, ←14, 8,	Ground	E	0					14 761.60	.1	214[1]
		15,10, ←16, 9,	Ground	E	0					19 608.29	.1	214[1]
		15,10, ←16, 9,	Ground	E	0					19 608.64	.1	214[1]
		15,10, ←16, 9,	Ground	A	0					19 609.28	.1	214[1]
		16, 7, ←15, 8,	Ground	A	0					27 575.98	.1	214[1]
		16, 7, ←15, 8,	Ground	E	0					27 576.76	.1	214[1]
		17, 8, ←16, 9,	Ground	A	0					16 721.31	.1	214[1]
		17, 8, ←16, 9,	Ground	E	0					16 722.23	.1	214[1]
		17,11, ←18,10,	Ground	E	0					17 645.83	.1	214[1]
		17,11, ←18,10,	Ground	E	0					17 646.35	.1	214[1]
		17,11, ←18,10,	Ground	A	0					17 646.86	.1	214[1]
		18, 8, ←17, 9,	Ground	A	0					29 530.32	.1	214[1]

1. See footnote preceding page.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	18, 8, ←17, 9,	Ground	E	1					29 531.24	.1	214[1]
		19, 9, ←18,10,	Ground	A	0					18 682.74	.1	214[1]
		19, 9, ←18,10,	Ground	E	0					18 683.46	.1	214[1]
		19, 9, ←18,10,	Ground	E	0					18 683.77	.1	214[1]
		19,12, ←20,11,	Ground	E	0					15 681.55	.1	214[1]
		19,12, ←20,11,	Ground	A	0					15 682.39	.1	214[1]
		20, 9, ←19,10,	Ground	A	0					31 486.76	.1	214[1]
		20, 9, ←19,10,	Ground	E	0					31 487.41	.1	214[1]
		20, 9, ←19,10,	Ground	E	0					31 487.79	.1	214[1]
		21,10, ←20,11,	Ground	A	0					20 644.92	.1	214[1]
		21,10, ←20,11,	Ground	E	0					20 645.46	.1	214[1]
		21,10, ←20,11,	Ground	E	0					20 645.91	.1	214[1]
		21,13, ←22,12,	Ground	E	0					13 715.56	.1	214[1]
		21,13, ←22,12,	Ground	A	0					13 716.40	.1	214[1]
		22,10, ←21,11,	Ground	A	0					33 444.73	.1	214[1]
		22,10, ←21,11,	Ground	E	0					33 445.03	.1	214[1]
		22,10, ←21,11,	Ground	E	0					33 445.65	.1	214[1]
		22,14, ←23,13,	Ground	E	0					24 484.77	.1	214[1]
		22,14, ←23,13,	Ground	A	0					24 485.56	.1	214[1]
		23,11, ←22,12,	Ground	A	0					22 607.49	.1	214[1]
		23,11, ←22,12,	Ground	E	0					22 607.74	.1	214[1]
		23,11, ←22,12,	Ground	E	0					22 608.43	.1	214[1]
		23,14, ←24,13,	Ground	E	0					11 747.79	.1	214[1]
		23,14, ←24,13,	Ground	A	0					11 748.57	.1	214[1]
		23,15, ←24,14,	Ground	E	0					35 237.97	.1	214[1]
		23,15, ←24,14,	Ground	A	0					35 238.67	.1	214[1]
		23,15, ←24,14,	Ground	E	0					35 238.97	.1	214[1]
		24,11, ←23,12,	Ground	A	0					35 402.99	.1	214[1]
		24,11, ←23,12,	Ground	E	0					35 403.15	.1	214[1]
		24,11, ←23,12,	Ground	E	0					35 403.83	.1	214[1]
		25,12, ←24,13,	Ground	A	0					24 570.46	.1	214[1]
		25,12, ←24,13,	Ground	E	0					24 571.27	.1	214[1]
		26,12, ←25,13,	Ground	A	0					37 361.64	.1	214[1]
		26,12, ←25,13,	Ground	E	0					37 362.45	.1	214[1]
		26,13, ←25,14,	Ground	A	0					13 759.98	.1	214[1]
		26,13, ←25,14,	Ground	E	0					13 760.70	.1	214[1]
		27,15, ←26,14,	Ground	A	0					26 533.12	.1	214[1]
		27,15, ←26,14,	Ground	E	0					26 533.80	.1	214[1]
		28,13, ←27,14,	Ground	A	0					39 320.40	.1	214[1]
		28,13, ←27,14,	Ground	E	0					39 321.14	.1	214[1]
		28,14, ←27,15,	Ground	E	0					15 725.83	.1	214[1]
		28,14, ←27,15,	Ground	A	0					15 725.98	.1	214[1]
		28,14, ←27,15,	Ground	E	0					15 726.58	.1	214[1]
		29,14, ←28,15,	Ground	E	0					28 496.04	.1	214[1]
		29,14, ←28,15,	Ground	A	0					28 496.19	.1	214[1]
		29,14, ←28,15,	Ground	E	0					28 496.98	.1	214[1]
		30,14, ←29,15,	Ground	A	0					41 279.30	.1	214[1]
		30,14, ←29,15,	Ground	E	0					41 279.97	.1	214[1]
		30,15, ←29,16,	Ground	E	0					17 692.15	.1	214[1]
		30,15, ←29,16,	Ground	A	0					17 692.55	.1	214[1]

1. In the labeling of transitions, the K_{+1} subscript has been omitted whenever the asymmetry splitting of the rotational levels is less than .1 MHz.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	30,15, ←29,16,	Ground	E	0					17 692.97	.1	214[1]
		31,15, ←30,16,	Ground							30 459.2	.1	214[1]
		32,16, ←31,17,	Ground	E	0					19 658.93	.1	214[1]
		32,16, ←31,17,	Ground	A	0					19 659.50	.1	214[1]
		32,16, ←31,17,	Ground	E	0					19 659.80	.1	214[1]
		33,16, ←32,17,	Ground	E	0					32 422.30	.1	214[1]
		33,16, ←32,17,	Ground	A	0					32 422.83	.1	214[1]
		33,16, ←32,17,	Ground	E	0					32 423.09	.1	214[1]
		34,17, ←33,18,	Ground	E	0					21 625.78	.1	214[1]
		34,17, ←33,18,	Ground	A	0					21 626.39	.1	214[1]
		35,17, ←34,18,	Ground	E	0					34 385.90	.1	214[1]
		35,17, ←34,18,	Ground	A	0					34 386.62	.1	214[1]
		36,18, ←35,19,	Ground	E	0					23 593.09	.1	214[1]
		36,18, ←35,19,	Ground	E	0					23 593.50	.1	214[1]
		36,18, ←35,19,	Ground	A	0					23 594.05	.1	214[1]
		37,18, ←36,19,	Ground	E	0					36 348.78	.1	214[1]
		37,18, ←36,19,	Ground	A	0					36 349.51	.1	214[1]
		38,19, ←37,20,	Ground	E	0					25 560.73	.1	214[1]
		38,19, ←37,20,	Ground	A	0					25 561.43	.1	214[1]
		39,19, ←38,20,	Ground	E	0					38 312.52	.1	214[1]
		39,19, ←38,20,	Ground	E	0					38 313.08	.1	214[1]
		39,19, ←38,20,	Ground	A	0					38 313.23	.1	214[1]
		40,20, ←39,21,	Ground	E	0					27 528.39	.1	214[1]
		40,20, ←39,21,	Ground	E	0					27 528.84	.1	214[1]
		40,20, ←39,21,	Ground	A	0					27 529.07	.1	214[1]
		41,20, ←40,21,	Ground	E	0					40 275.31	.1	214[1]
		41,20, ←40,21,	Ground	A	0					40 276.05	.1	214[1]
		42,21, ←41,22,	Ground	E	0					29 496.35	.1	214[1]
		42,21, ←41,22,	Ground	E	0					29 496.60	.1	214[1]
		42,21, ←41,22,	Ground	A	0					29 497.04	.1	214[1]
		44,22, ←43,23,	Ground	E	0					31 464.36	.1	214[1]
		44,22, ←43,23,	Ground	A	0					31 464.96	.1	214[1]
		46,23, ←45,24,	Ground	E	0					33 432.64	.1	214[1]
		46,23, ←45,24,	Ground	A	0					33 433.28	.1	214[1]
		48,24, ←47,25,	Ground	E	0					35 400.94	.1	214[1]
		48,24, ←47,25,	Ground	A	0					35 401.45	.1	214[1]
		Not Reported	Ground							9 797.13	.1	214
		Not Reported	Ground							9 798.95	.1	214
		Not Reported	Ground							9 799.75	.1	214
		Not Reported	Ground							10 786.85	.1	214
		Not Reported	Ground							10 816.43	.1	214
		Not Reported	Ground							10 939.88	.1	214
		Not Reported	Ground							11 087.72	.1	214
		Not Reported	Ground							11 466.80	.1	214
		Not Reported	Ground							12 596.59	.1	214
		Not Reported	Ground							13 273.35	.1	214
		Not Reported	Ground							13 279.04	.1	214
		Not Reported	Ground							14 053.63	.1	214
		Not Reported	Ground							14 739.48	.1	214
		Not Reported	Ground							14 756.47	.1	214

1. See footnote preceding page.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{*}HO^{16}C^{12}{*}H_2$	761	Not Reported	Ground						15 731.38	.1	214
		Not Reported	Ground						15 756.36	.1	214
		Not Reported	Ground						17 986.82	.1	214
		Not Reported	Ground						18 028.11	.1	214
		Not Reported	Ground						18 043.35	.1	214
		Not Reported	Ground						19 602.38	.1	214
		Not Reported	Ground						19 660.31	.1	214
		Not Reported	Ground						20 545.78	.1	214
		Not Reported	Ground						20 942.26	.1	214
		Not Reported	Ground						20 953.54	.1	214
		Not Reported	Ground						21 019.01	.1	214
		Not Reported	Ground						21 060.27	.1	214
		Not Reported	Ground						21 346.97	.1	214
		Not Reported	Ground						23 946.91	.1	214
		Not Reported	Ground						23 951.99	.1	214
		Not Reported	Ground						24 034.84	.1	214
		Not Reported	Ground						24 678.02	.1	214
		Not Reported	Ground						25 145.18	.1	214
		Not Reported	Ground						25 149.28	.1	214
		Not Reported	Ground						25 159.28	.1	214
		Not Reported	Ground						25 222.45	.1	214
		Not Reported	Ground						25 637.07	.1	214
		Not Reported	Ground						26 916.24	.1	214
		Not Reported	Ground						26 927.34	.1	214
		Not Reported	Ground						27 127.45	.1	214
		Not Reported	Ground						27 138.22	.1	214
		Not Reported	Ground						27 159.69	.1	214
		Not Reported	Ground						27 186.05	.1	214
		Not Reported	Ground						27 196.07	.1	214
		Not Reported	Ground						27 241.74	.1	214
		Not Reported	Ground						27 432.92	.1	214
		Not Reported	Ground						28 421.47	.1	214
		Not Reported	Ground						28 863.35	.1	214
		Not Reported	Ground						28 955.44	.1	214
		Not Reported	Ground						28 975.36	.1	214
		Not Reported	Ground						29 069.38	.1	214
		Not Reported	Ground						29 123.46	.1	214
		Not Reported	Ground						29 213.55	.1	214
		Not Reported	Ground						29 370.43	.1	214
		Not Reported	Ground						29 371.74	.1	214
		Not Reported	Ground						29 373.24	.1	214
		Not Reported	Ground						29 499.04	.1	214
		Not Reported	Ground						29 604.65	.1	214
		Not Reported	Ground						29 684.32	.1	214
		Not Reported	Ground						30 434.95	.1	214
		Not Reported	Ground						30 438.57	.1	214
		Not Reported	Ground						30 835.45	.1	214
		Not Reported	Ground						31 025.99	.1	214
		Not Reported	Ground						31 026.88	.1	214
		Not Reported	Ground						31 031.88	.1	214

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*HO^{16}C^{12}{}_*H_2$	761	Not Reported	Ground						31 034.24	.1	214
		Not Reported	Ground						31 167.79	.1	214
		Not Reported	Ground						31 168.63	.1	214
		Not Reported	Ground						31 299.81	.1	214
		Not Reported	Ground						31 300.41	.1	214
		Not Reported	Ground						31 465.89	.1	214
		Not Reported	Ground						32 332.64	.1	214
		Not Reported	Ground						32 847.29	.1	214
		Not Reported	Ground						32 848.94	.1	214
		Not Reported	Ground						32 948.69	.1	214
		Not Reported	Ground						32 974.99	.1	214
		Not Reported	Ground						33 141.61	.1	214
		Not Reported	Ground						33 216.01	.1	214
		Not Reported	Ground						34 070.35	.1	214
		Not Reported	Ground						34 187.18	.1	214
		Not Reported	Ground						34 200.10	.1	214
		Not Reported	Ground						34 262.44	.1	214
		Not Reported	Ground						34 306.81	.1	214
		Not Reported	Ground						34 310.92	.1	214
		Not Reported	Ground						34 572.69	.1	214
		Not Reported	Ground						34 722.92	.1	214
		Not Reported	Ground						35 571.32	.1	214
		Not Reported	Ground						35 776.82	.1	214
		Not Reported	Ground						35 840.37	.1	214
		Not Reported	Ground						36 211.58	.1	214
		Not Reported	Ground						36 831.82	.1	214
		Not Reported	Ground						37 610.25	.1	214
		Not Reported	Ground						37 617.40	.1	214
		Not Reported	Ground						37 658.65	.1	214
		Not Reported	Ground						37 660.53	.1	214
		Not Reported	Ground						37 698.01	.1	214
		Not Reported	Ground						37 769.29	.1	214
		Not Reported	Ground						37 782.96	.1	214
		Not Reported	Ground						37 791.71	.1	214
		Not Reported	Ground						37 799.76	.1	214
		Not Reported	Ground						37 841.92	.1	214
		Not Reported	Ground						37 870.87	.1	214
		Not Reported	Ground						37 879.45	.1	214
		Not Reported	Ground						37 953.44	.1	214
		Not Reported	Ground						37 985.33	.1	214
		Not Reported	Ground						38 762.75	.1	214
		Not Reported	Ground						38 836.98	.1	214
		Not Reported	Ground						38 861.90	.1	214
		Not Reported	Ground						38 989.23	.1	214
		Not Reported	Ground						39 000.03	.1	214
		Not Reported	Ground						39 003.23	.1	214

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C_3H_7Cl $C_s(C_{3v},C_{2v},C_s)$ C_3H_7Cl

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
t-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{35}$	C_s	771		2 379.7 M	2 271.7 M				
t-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{37}$	C_s	772		2 325.8 M	2 222.4 M				
g-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{35}$	C_1	773	11 829.22 M	3 322.58 M	2 853.06 M				
g-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{37}$	C_1	774	11 788.12 M	3 249.02 M	2 796.44 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
771	2.05 T		0. X		3250						

References:

ABC: 365 D_J: D_{JK}: κ: Δ:

μ: 393 eQq: V: 365 I: ω:

Add. Ref.: 388

1-Chloropropane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
t-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{35}$	771	4, 1, 3← 3, 1, 2	Ground	A	0					18 820.72	.2	365
		4, 1, 4← 3, 1, 3	Ground	A	0					18 389.10	.2	365
		5, 1, 4← 4, 1, 3	Ground	A	0					23 525.21	.2	365
		5, 1, 5← 4, 1, 4	Ground	A	0					22 985.16	.2	365
		6, 1, 5← 5, 1, 4	Ground	A	0					28 228.93	.2	365
		6, 1, 6← 5, 1, 5	Ground	A	0					27 580.96	.2	365
t-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{37}$	772	4, 1, 3← 3, 1, 2	Ground	A	0					18 398.68	.2	365
		4, 1, 4← 3, 1, 3	Ground	A	0					17 985.71	.2	365
		5, 1, 4← 4, 1, 3	Ground	A	0					22 998.38	.2	365
		5, 1, 5← 4, 1, 4	Ground	A	0					22 480.92	.2	365
		6, 1, 5← 5, 1, 4	Ground	A	0					27 596.50	.2	365
		6, 1, 6← 5, 1, 5	Ground	A	0					26 976.65	.2	365
g-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{35}$	773	1, 1, 1← 0, 0, 0	Ground	A	0					14 682.93	.2	365
		2, 1, 2← 1, 0, 1	Ground	A	0					20 388.94	.2	365
		2, 1, 1← 1, 1, 0	Ground	A	0					12 820.80	.2	365
		2, 1, 2← 1, 1, 1	Ground	A	0					11 881.80	.2	365
		3, 0, 3← 2, 0, 2	Ground	A	0					18 450.95	.2	365
		3, 1, 2← 2, 1, 1	Ground	A	0					19 218.84	.2	365
		3, 1, 3← 2, 1, 2	Ground	A	0					17 810.83	.2	365
		4, 0, 4← 3, 0, 3	Ground	A	0					24 514.76	.2	365
		4, 1, 3← 3, 1, 2	Ground	A	0					25 601.63	.2	365
		4, 1, 4← 3, 1, 3	Ground	A	0					23 726.51	.2	365
		4, 2, 2← 3, 2, 1	Ground	A	0					24 874.53	.2	365
		4, 2, 3← 3, 2, 2	Ground	A	0					24 687.66	.2	365
		4, 2, 2← 4, 1, 3	Ground	A	0					24 196.71	.2	365
		5, 0, 5← 4, 0, 4	Ground	A	0					30 507.94	.2	365
		5, 1, 4← 4, 1, 3	Ground	A	0					31 962.82	.2	365

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
g-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{35}$	773	5, 1, 5← 4, 1, 4	Ground	A	0					29 625.73	.2	365
		5, 2, 3← 4, 2, 2	Ground	A	0					31 204.35	.2	365
		5, 2, 4← 4, 2, 3	Ground	A	0					30 835.52	.2	365
		5, 2, 3← 5, 1, 4	Ground	A	0					23 438.25	.2	365
		6, 2, 4← 6, 1, 5	Ground	A	0					22 739.83	.2	365
		7, 2, 5← 7, 1, 6	Ground	A	0					22 198.83	.2	365
		8, 1, 7← 8, 0, 8	Ground	A	0					19 801.74	.2	365
		8, 2, 6← 8, 1, 7	Ground	A	0					21 908.77	.2	365
		9, 1, 8← 9, 0, 9	Ground	A	0					23 101.55	.2	365
		9, 2, 7← 9, 1, 8	Ground	A	0					21 953.55	.2	365
		10, 1, 9←10, 0,10	Ground	A	0					26 847.33	.2	365
		10, 2, 8←10, 1, 9	Ground	A	0					22 404.11	.2	365
		11, 1,10←11, 0,11	Ground	A	0					30 975.79	.2	365
		11, 2, 9←11, 1,10	Ground	A	0					23 319.44	.2	365
		12, 2,10←12, 1,11	Ground	A	0					24 747.74	.2	365
		13, 2,11←13, 1,12	Ground	A	0					26 726.06	.2	365
		14, 2,12←14, 1,13	Ground	A	0					29 275.28	.2	365
		15, 2,13←15, 1,14	Ground	A	0					32 394.45	.2	365
g-$C^{12}H_3C^{12}H_2C^{12}H_2Cl^{37}$	774	2, 1, 2← 1, 0, 1	Ground	A	0					20 177.44	.2	365
		3, 0, 3← 2, 0, 2	Ground	A	0					18 066.55	.2	365
		3, 1, 2← 2, 1, 1	Ground	A	0					18 804.10	.2	365
		3, 1, 3← 2, 1, 2	Ground	A	0					17 466.78	.2	365
		4, 0, 4← 3, 0, 3	Ground	A	0					24 007.67	.2	365
		4, 1, 3← 3, 1, 2	Ground	A	0					25 050.53	.2	365
		4, 1, 4← 3, 1, 3	Ground	A	0					23 242.41	.2	365
		4, 2, 2← 3, 2, 1	Ground	A	0					24 344.40	.2	365
		4, 2, 3← 3, 2, 2	Ground	A	0					24 168.19	.2	365
		4, 2, 2← 4, 1, 3	Ground	A	0					24 327.14	.2	365
		5, 0, 5← 4, 0, 4	Ground	A	0					29 883.72	.2	365
		5, 1, 4← 4, 1, 3	Ground	A	0					31 275.86	.2	365
		5, 1, 5← 4, 1, 4	Ground	A	0					29 022.88	.2	365
		5, 2, 3← 4, 2, 2	Ground	A	0					30 530.25	.2	365
		5, 2, 4← 4, 2, 3	Ground	A	0					30 187.94	.2	365
		5, 2, 3← 5, 1, 4	Ground	A	0					23 581.92	.2	365
		6, 2, 4← 6, 1, 5	Ground	A	0					22 883.98	.2	365
		7, 2, 5← 7, 1, 6	Ground	A	0					22 326.14	.2	365
		8, 1, 7← 8, 0, 8	Ground	A	0					19 352.82	.2	365
		8, 2, 6← 8, 1, 7	Ground	A	0					21 996.93	.2	365
		9, 1, 8← 9, 0, 9	Ground	A	0					22 514.93	.2	365
		9, 2, 7← 9, 1, 8	Ground	A	0					21 987.43	.2	365
		10, 1, 9←10, 0,10	Ground	A	0					26 115.03	.2	365
		10, 2, 8←10, 1, 9	Ground	A	0					22 339.23	.2	365
		11, 1,10←11, 0,11	Ground	A	0					30 098.56	.2	365
		11, 2, 9←11, 1,10	Ground	A	0					23 137.29	.2	365
		12, 2,10←12, 1,11	Ground	A	0					24 420.34	.2	365
		14, 2,12←14, 1,13	Ground	A	0					28 578.27	.2	365
		15, 2,13←15, 1,14	Ground	A	0					31 482.71	.2	365

C_3H_8 $C_{2v}(C_{3v},C_{2v},C_{3v})$ $CH_3CH_2CH_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H_2C^{12}H_3$	C_{2v}	781	29 207.36 M	8 446.07 M	7 458.98 M		<.05		
$C^{13}H_3C^{12}H_2C^{12}H_3$	C_s	782	29 092.05 M	8 228.77 M	7 281.73 M				
$C^{12}H_3C^{13}H_2C^{12}H_3$	C_{2v}	783	28 660.50 M	8 447.11 M	7 423.19 M				
$C^{12}H_3C^{12}HDC^{12}H_3$	C_1	784	25 829.94 M	8 358.76 M	7 283.00 M				
s-$C^{12}DH_2C^{12}H_2C^{12}H_3$	C_s	785	29 017.79 M	7 838.32 M	6 971.96 M				
a-$C^{12}H_2DC^{12}H_2C^{12}H_3$	C_1	786	26 828.97 M	8 123.10 M	7 185.14 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
781	0. X	0.083 M	0. X		3400						

References:

ABC: 296 D_J: D_{JK}: 296 κ: Δ:

μ: 296 eQq: V: 113 I: ω:

Add. Ref.: 146

Torsional frequency = 250 cm^{-1}. Ref: 296.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H_2C^{12}H_3$	781	1, 1, 1← 0, 0, 0	Ground						36 666.33	.06	296
		1, 1, 0← 1, 0, 1	Ground						21 748.37	.03	296
		2, 1, 1← 2, 0, 2	Ground						22 769.74	.03	296
		3, 1, 2← 3, 0, 3	Ground						24 365.47	.03	296
		4, 1, 3← 4, 0, 4	Ground						26 609.24	.03	296
		5, 1, 4← 5, 0, 5	Ground						29 592.51	.03	296
		6, 1, 5← 6, 0, 6	Ground						33 414.72	.03	296
$C^{13}H_3C^{12}H_2C^{12}H_3$	782	1, 1, 1← 0, 0, 0	Ground						36 373.78	.12	296
		2, 1, 1← 2, 0, 2	Ground						22 788.80	.06	296
		3, 1, 2← 3, 0, 3	Ground						24 315.01	.06	296
		4, 1, 3← 4, 0, 4	Ground						26 456.74	.06	296
		5, 1, 4← 5, 0, 5	Ground						29 298.58	.06	296
		6, 1, 5← 6, 0, 6	Ground						32 933.58	.06	296
$C^{12}H_3C^{13}H_2C^{12}H_3$	783	1, 1, 1← 0, 0, 0	Ground						36 083.69	.12	296
		2, 1, 1← 2, 0, 2	Ground						22 299.03	.06	296
		3, 1, 2← 3, 0, 3	Ground						23 961.76	.06	296
		4, 1, 3← 4, 0, 4	Ground						26 306.35	.06	296
		5, 1, 4← 5, 0, 5	Ground						29 432.48	.06	296
		6, 1, 5← 6, 0, 6	Ground						33 446.47	.06	296
$C^{12}H_3C^{12}HDC^{12}H_3$	784	1, 1, 1← 0, 0, 0	Ground						33 112.93	.12	296
		2, 1, 1← 2, 0, 2	Ground						19 670.78	.06	296
		3, 1, 2← 3, 0, 3	Ground						21 445.48	.06	296
		4, 1, 3← 4, 0, 4	Ground						23 971.76	.06	296
		5, 1, 4← 5, 0, 5	Ground						27 370.09	.06	296
		6, 1, 5← 6, 0, 6	Ground						31 759.70	.06	296
s-$C^{12}DH_2C^{12}H_2C^{12}H_3$	785	1, 1, 1← 0, 0, 0	Ground						35 989.76	.12	296
		2, 1, 1← 2, 0, 2	Ground						22 938.16	.06	296
		3, 1, 2← 3, 0, 3	Ground						24 324.96	.06	296
		4, 1, 3← 4, 0, 4	Ground						26 262.62	.06	296
		5, 1, 4← 5, 0, 5	Ground						28 822.23	.06	296
		6, 1, 5← 6, 0, 6	Ground						32 083.91	.06	296
a-$C^{12}H_2DC^{12}H_2C^{12}H_3$	786	1, 1, 1← 0, 0, 0	Ground						34 014.10	.12	296
		2, 1, 1← 2, 0, 2	Ground						20 616.12	.06	296
		3, 1, 2← 3, 0, 3	Ground						22 137.98	.06	296
		4, 1, 3← 4, 0, 4	Ground						24 283.11	.06	296
		5, 1, 4← 5, 0, 5	Ground						27 141.90	.06	296
		6, 1, 5← 6, 0, 6	Ground						30 811.32	.06	296

C_3H_9As $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3As$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3As^{75}$	C_{3v}	791	4 724.98 M	4 724.98 M		.003			

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
791	0. X	0. X	0.86 M	−203.2	2000	500					

References:

ABC: 254 D_J: 254 D_{JK}: κ: Δ:

μ: 254 eQq: 254 V: 254 I: ω:

Rotational constant for the excited state: $B_V = 4748.9$ MHz. Ref: 254.

Trimethylarsine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_I'	Hyperfine F'	Hyperfine F_I	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3As^{75}$	791	2, 0← 1, 0	Ground			5/2		3/2	18 904.22	.05	254
		2, 0← 1, 0	Ground			7/2		5/2	18 904.22	.05	254
		2, 1← 1, 1	Ground			5/2		3/2	18 861.48	.05	254
		2, 1← 1, 1	Ground			5/2		5/2	18 886.8		254
		2, 1← 1, 1	Ground			7/2		5/2	18 912.15	.05	254
		2, 1← 1, 1	Ground			3/2		1/2	18 925.3		254
		3, 0← 2, 0	Ground			7/2		7/2	28 302.		254
		3, 0← 2, 0	Ground			5/2		3/2	28 339.44	.05	254
		3, 0← 2, 0	Ground			3/2		1/2	28 339.44	.05	254
		3, 0← 2, 0	Ground			7/2		5/2	28 351.95	.05	254
		3, 0← 2, 0	Ground			9/2		7/2	28 351.95	.05	254
		3, 0← 2, 0	Ground			3/2		3/2	28 390.13	.05	254
		3, 1← 2, 1	Ground			7/2		7/2	28 316.95	.05	254
		3, 1← 2, 1	Ground			7/2		5/2	28 342.11	.05	254
		3, 1← 2, 1	Ground			5/2		3/2	28 342.11	.05	254
		3, 1← 2, 1	Ground			3/2		1/2	28 354.93	.05	254
		3, 1← 2, 1	Ground			9/2		7/2	28 354.93	.05	254
		3, 1← 2, 1	Ground			5/2		5/2	28 360.04	.05	254
		3, 1← 2, 1	Ground			3/2		3/2	28 380.00	.05	254
		3, 2← 2, 2	Ground			5/2		5/2	28 313.36	.05	254
		3, 2← 2, 2	Ground			7/2		5/2	28 313.36	.05	254
		3, 2← 2, 2	Ground			3/2		3/2	28 349.62	.05	254
		3, 2← 2, 2	Ground			5/2		3/2	28 349.62	.05	254
		3, 2← 2, 2	Ground			7/2		7/2	28 364.13	.05	254
		3, 2← 2, 2	Ground			9/2		7/2	28 364.13	.05	254
		3, 2← 2, 2	Ground			1/2		1/2	28 400.43	.05	254
		3, 2← 2, 2	Ground			3/2		1/2	28 400.43	.05	254

$C_3H_9BF_3N$ $C_{3v}(C_{3v},C_{3v},C_{3v},C_{3v},C_{3v},C_{3v})$ $F_3B{\cdot}N(CH_3)_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$F_3^{19}B^b{\cdot}N^b(C^{12}H_3)_3$	C_{3v}	801		1 750. [2]M					

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
801	5. [1]M	0. X	0. X								

1. Since it is not stated whether this molecule is a prolate or oblate top, the total dipole moment may be entered under either μ_a or μ_c. For convenience, it has been entered here as μ_a.

2. Measurements were made on a mixture of isotopes, B^{11} (81%) and B^{10} (19%). Either B = C (prolate) or A = B (oblate).

References:

ABC: 308 D_J: D_{JK}: κ: Δ:

μ: 308 eQq: V: I: ω:

Trifluoroborane-trimethylamine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$F_3^{19}B^b{\cdot}N^b(C^{12}H_3)_3$	801	2, ← 1,							6 990.		308[1]
		3, ← 2,							10 480.		308[1]
		9, ← 8,							31 500.		308[1]
		10, ← 9,							35 000.		308[1]

1. The values given are average frequencies of broad unresolved lines of varying widths.

C_3H_9BrSi $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3SiBr$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3Si^{28}Br^{79}$	C_{3v}	811		1 461.95 M	1 461.95 M				
$(C^{12}H_3)_3Si^{28}Br^{81}$	C_{3v}	812		1 449.13 M	1 449.13 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
811	2.36 L	0. X	0. X								

References:

ABC: 149 D_J: D_{JK}: κ: Δ:

μ: 372 eQq: V: I: ω:

Add. Ref.: 104

Trimethylbromosilane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3Si^{28}Br^{79}$	811	10, ← 9,	Ground						29 238.7	.3	149
		11, ←10,							32 112.2	.4	149
		11, ←10,							32 124.6	.4	149
		11, ←10,							32 139.0	.4	149
		11, ←10,	Ground						32 162.0	.3	149
		11, ←10,							32 194.3	.4	149
		11, ←10,							32 202.2	.4	149
		12, ←11,							35 032.9	.4	149
		12, ←11,							35 045.8	.4	149
		12, ←11,							35 061.2	.4	149
		12, ←11,	Ground						35 087.4	.3	149
		12, ←11,							35 121.9	.4	149
		13, ←12,	Ground						38 010.8	.3	149
$(C^{12}H_3)_3Si^{28}Br^{81}$	812	10, ← 9,	Ground						28 982.5	.3	149
		11, ←10,							31 831.6	.4	149
		11, ←10,							31 842.1	.4	149
		11, ←10,							31 856.2	.4	149
		11, ←10,	Ground						31 880.5	.3	149
		11, ←10,							31 913.2	.4	149
		11, ←10,							31 920.2	.4	149
		12, ←11,							34 725.2	.4	149
		12, ←11,							34 736.9	.4	149
		12, ←11,							34 753.2	.4	149
		12, ←11,	Ground						34 779.1	.3	149
		12, ←11,							34 814.1	.4	149
		12, ←11,							34 822.4	.4	149
		13, ←12,	Ground						37 675.3	.4	149
		14, ←13,	Ground						40 575.5	.3	149

C_3H_9ClSi $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3Si$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3Si^{28}Cl^{35}$	C_{3v}	821		2 197.441 M	2 197.441 M		<.010		
$(C^{12}H_3)_3Si^{28}Cl^{37}$	C_{3v}	822		2 147.883 M	2 147.883 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
821	2.02 L	0. X	0. X								

References:

ABC: 79, 303 D_J: D_{JK}: 79 κ: Δ:

μ: 167 eQq: V: I: ω:

Add. Refs.: 80, 85

Trimethylchlorosilane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3Si^{28}Cl^{35}$	821	5, ← 4,	Ground						21 974.00	.3	79
		7, ← 6,	Ground						30 762.89	.2	79
		8, ← 7,	Excited						35 107.16	.3	79
		8, ← 7,	Excited						35 133.71	.3	79
		8, ← 7,	Ground						35 157.01	.3	79
		8, ← 7,	Excited						35 198.47	.3	79
		8, ← 7,	Excited						35 219.92	.3	79
		9, ← 8,	Excited						39 524.50	.3	79
		9, ← 8,	Excited						39 550.89	.3	79
		9, ← 8,	Excited						39 597.95	.3	79
		9, ← 8,	Excited						39 622.21	.3	79
$(C^{12}H_3)_3Si^{28}Cl^{37}$	822	8, ← 7,	Excited						34 317.44	.5	79
		8, ← 7,	Excited						34 343.20	.5	79
		8, ← 7,	Ground						34 366.12	.5	79
		8, ← 7,	Excited						34 406.36	.5	79
		8, ← 7,	Excited						34 426.86	.5	79
		9, ← 8,	Excited						38 607.26	.5	79
		9, ← 8,	Excited						38 636.09	.5	79
		9, ← 8,	Excited						38 662.28	.5	79
		9, ← 8,	Excited						38 707.44	.5	79
		9, ← 8,	Excited						38 731.09	.5	79

C_3H_9FSi $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3SiF$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3Si^{28}F^{19}$	C_{3v}	831		3 411.00 M	3 411.00 M				

References:

ABC: 88 D_J: D_{JK}: κ: Δ:

μ: eQq: V: I: ω:

Add. Ref.: 219

Trimethylfluorosilane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3Si^{28}F^{19}$	831	4, ← 3,	Ground						27 287.8	.3	88
		5, ← 4,	Excited						34 088.6	.5	88
		5, ← 4,	Excited						34 094.9	.5	88
		5, ← 4,	Ground						34 109.8	.3	88
		5, ← 4,	Excited						34 133.4	.3	88
		5, ← 4,	Excited						34 148.		88
		5, ← 4,	Excited						34 171.		88
		5, ← 4,	Excited						34 219.0	.5	88
		6, ← 5,	Excited						40 906.3	.3	88
		6, ← 5,	Excited						40 913.0	.5	88
		6, ← 5,	Ground						40 931.6	.3	88
		6, ← 5,	Excited						40 959.4	.5	88
		6, ← 5,	Excited						40 977.		88
		6, ← 5,	Excited						41 008.		88
		6, ← 5,	Excited						41 062.5	.5	88

840 - Trimethyliodosilane
Trimethyliodosilicane

Molecular Constant Table

C_3H_9ISi $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3SiI$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3Si^{28}I^{127}$	C_{3v}	841		1 096.42 M	1 096.42 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{rcd}	ω_a d	ω_b d	ω_c d	ω_d d
841	2.46 L	0. X	0. X								

References:

ABC: 152 D_J: D_{JK}: κ: Δ:

μ: 167 eQq: V: I: ω:

Add. Refs.: 104, 167

Trimethyliodosilane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_I'	Hyperfine F'	Hyperfine F_I	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3Si^{28}I^{127}$	841	15, ←14,	Excited						32 834.2	.4	152
		15, ←14,	Excited						32 847.4	.4	152
		15, ←14,	Excited						32 854.4	.4	152
		15, ←14,	Excited						32 874.3	.4	152
		15, ←14,	Ground						32 892.9	.3	152
		15, ←14,	Excited						32 917.2	.4	152
		15, ←14,	Excited						32 940.2	.4	152
		15, ←14,	Excited						32 948.9	.4	152
		16, ←15,	Excited						35 038.3	.4	152
		16, ←15,	Excited						35 044.9	.4	152
		16, ←15,	Excited						35 064.7	.4	152
		16, ←15,	Ground						35 085.2	.3	152
		16, ←15,	Excited						35 111.0	.4	152
		16, ←15,	Excited						35 136.4	.4	152
		16, ←15,	Excited						35 145.9	.4	152
		17, ←16,	Excited						37 210.6	.4	152
		17, ←16,	Excited						37 227.4	.4	152
		17, ←16,	Excited						37 234.7	.4	152
		17, ←16,	Excited						37 256.4	.4	152
		17, ←16,	Ground						37 278.0	.3	152
		17, ←16,	Excited						37 305.3	.4	152
		17, ←16,	Excited						37 331.7	.4	152
		17, ←16,	Excited						37 342.7	.4	152

C_3H_9N $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3N$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3N^{14}$	C_{3v}	851	8 720.86 M	8 720.86 M		.005	.000		
$(C^{12}H_3)_2C^{13}H_3N^{14}$	C_s	852	8 719.3 M	8 445.5 M	5 200. M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
851	0. X	0. X	0.612 M	−5.47	4400						

References:

ABC: 225 D_J: 225 D_{JK}: 225 κ: Δ:

μ: 225 eQq: 225 V: 225 I: ω:

Add. Refs.: 242, 282

Torsional frequencies: $A_2 = 263$ cm^{-1}, $E = 290$ cm^{-1}. Ref: 225. The A_2 mode is forbidden in both the infrared and Raman spectra, but a Raman line at 274 cm^{-1} may perhaps be identified with the E torsion.

Trimethylamine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3N^{14}$	851	1, ← 0,	Ground							17 375.0	.3	225[1]
		1, ← 0,	Ground							17 380.8	.3	225[1]
		1, ← 0,	Ground							17 387.9	.3	225[1]
		1, ← 0,	Ground	A	2					17 401.	1.	225[1]
		1, ← 0,	Ground	E	1					17 407.45	.10	225[1]
		1, 0,	Ground	A	1					17 421.41	.10	225[1]
		1, 0 0, 0	Ground				1		1	17 440.33		225
		1, 0,	Ground	A	0					17 441.71	.03	225[1]
		1, 0 0, 0	Ground				2		1	17 441.98		225
		1, 0 0, 0	Ground				0		1	17 444.43		225
		1, 0,	Excited							17 477.	1.	225[1]
		2, 1,	Ground							34 749.0	.3	225[1]
		2, 1,	Ground							34 760.9	.3	225[1]
		2, 1,	Ground	E	1					34 774.0	.3	225[1]
		2, 1,	Ground							34 775.7	.3	225[1]
		2, 1,	Ground	A	2					34 800.0	.3	225[1]
		2, 1,	Ground	E	1					34 814.84	.05	225[1]
		2, 1,	Ground	A	1					34 842.61	.05	225[1]
		2, 1,	Ground	E	1					34 855.4	.3	225[1]
		2, 0 1, 0	Ground				2		2	34 881.68		225
		2, 0 1, 0	Ground				1		0	34 881.94		225
		2, 0 1, 0	Ground	A	0					34 883.31	.03	225
		2, 0 1, 0	Ground				3		2	34 883.42		225
		2, 0 1, 0	Ground				1		1	34 886.04		225
		2, 1,	Excited							34 955.6	.3	225[1]
		2, 1 1, 1	Ground				2		1	34 881.94		225
		2, 1 1, 1	Ground				2		2	34 882.79		225
		2, 1 1, 1	Ground	A	0					34 883.32	.03	225
		2, 1 1, 1′	Ground				3		2	34 883.65		225
		2, 1 1, 1	Ground				1		0	34 885.38		225
$(C^{12}H_3)_2C^{13}H_3N^{14}$	852	1, 1, 0← 0, 0, 0	Ground							17 165.0	.5	225
		2, 1, 1← 1, 0, 1	Ground							34 055.7	.5	225
		2, 2, 0← 1, 1, 0	Ground							34 346.2	.2	225
		2, 2, 1← 1, 1, 1	Ground							34 603.5	.5	225

1. A possible but not certain identification of some of the torsional satellites is made in Table II of Lide's paper. Also a tentative identification of two non-torsional excited vibrational states is made in the same table.

C_3H_9P $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3P$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3P^{31}$	C_{3v}	861	5 816.24 M	5 816.24 M		.003			
$C^{13}H_3(C^{12}H_3)_2P^{31}$	C_s	862	5 809.07 M	5 640.73 M	3 669. M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
861	0. X	0. X	1.192 M		2600			316[1] 1	253[1] 2		

1. The vibrational frequencies for the low lying δ_a and δ_c vibrational modes by microwave analysis are in Lide and Mann's article on isobutane, and it is shown that the previous IR or Raman identifications for these modes should be reversed.

References:

ABC: 226 D_J: 226 D_{JK}: κ: Δ:

μ: 226 eQq: V: 226 I: ω: 226

Rotational Constants for excited states (B_V): τ_a: 5809.91 MHz; τ_c: 5806.49 MHz; δ_a: 5823.94 MHz; δ_c: 5817.80. Torsional frequencies: τ_a: 197 ± 20 cm^{-1}; τ_c: 223 ± 20 cm^{-1}. Ref: 226.

Trimethylphosphine

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3P^{31}$	861	2, ← 1,	Ground	E 1					23 225.87		226
		2, ← 1,	Ground	A 1					23 239.54		226
		2, ← 1,	Ground						23 264.86	.03	226
		2, ← 1,							23 271.20		226
		2, ← 1,	1						23 295.71		226
		2, 1← 1, 1	Excited	E 1					23 262.8		226[1]
		2, 1← 1, 1	Excited	E 1					23 188.65	.03	226[1]
		2, 1← 1, 1	Excited	E 1					23 225.87	.03	226[1]
		3, ← 2,	Ground	E 1					34 839.		226
		3, ← 2,	Ground	A 1					34 859.10		226
		3, ← 2,	Ground						34 897.11	.03	226
		3, ← 2,							34 907.		226
		3, ← 2,	1						34 943.46		226
		3, 0← 2, 0	Excited	E 1					34 839.96	.03	226[1]
		3, 1← 2, 1	Excited	E 1					34 894.2		226[1]
		3, 1← 2, 1	Excited	E 1					34 782.7		226[1]
		3, 1← 2, 1	Excited	E 1					34 839.05	.03	226[1]
		3, 2← 2, 2	Excited	E 1					34 837.25	.03	226[1]
$C^{13}H_3(C^{12}H_3)_2P^{31}$	862	3, 1, 2← 2, 0, 2	Ground						34 308.4		226
		3, 2, 1← 2, 1, 1	Ground						34 103.5		226
		3, 2, 2← 2, 1, 2	Ground						34 349.3		226
		3, 3, 0← 2, 2, 0	Ground						34 390.5		226
		3, 3, 1← 2, 2, 1	Ground						34 608.1		226

1. *l*-doubling occurs here in the singly excited torsional state. A simple treatment of this is given in the reference by Lide and Mann.

$C_3H_{10}Si$ $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3SiH$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3Si^{28}H$	C_{3v}	871	5 345.15 M	5 345.15 M	3 166. M				
$(C^{12}H_3)_3Si^{28}D$	C_{3v}	872	5 159.71 M	5 159.71 M					
$(C^{12}H_3)_3Si^{29}H$	C_{3v}	873	5 337.84 M	5 337.84 M					
$(C^{12}H_3)_3Si^{29}D$	C_{3v}	874	5 153.87 M	5 153.87 M					
$(C^{12}H_3)_3Si^{30}H$	C_{3v}	875	5 330.84 M	5 330.84 M					
$(C^{12}H_3)_3Si^{30}D$	C_{3v}	876	5 148.13 M	5 148.13 M					
$C^{13}H_3(C^{12}H_3)_2Si^bH$	C_s	877	5 342.14 M	5 172.63 M	3 105. M				
$(C^{13}H_3)_2C^{12}H_3Si^bH$	C_s	878	5 254.02 M	5 086.00 M	3 135. M				
$(C^{12}D_3)_2C^{12}H_3Si^bH$	C_s	879	4 724.61 M	4 216.49 M	2 656. M				
s-$C^{12}H_2D(C^{12}H_3)_2Si^bD$	C_s	881	5 070.23 M	4 905.69 M	3 101. M				
a-$C^{12}H_2D(C^{12}H_3)_2Si^bD$	C_1	882	5 157.86 M	4 859.67 M	3 050. M				
s-$C^{12}D_2H(C^{12}H_3)_2Si^bD$	C_s	883	5 076.72 M	4 662.40 M	2 945. M				
a-$C^{12}D_2H(C^{12}H_3)_2Si^bD$	C_1	884	5 052.74 M	4 650.07 M	2 992. M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
871	0. X	0. X	0.525 M		1830	400					

References:

ABC: 307 D_J: D_{JK}: κ: Δ:

μ: 307 eQq: V: 307 I: ω:

Add. Ref.: 287

For species 879, the calculated torsional frequencies are: $\omega_2 = 104$ cm^{-1}, and $\omega_3 = 141$ cm^{-1}, and $\omega_3 = 141$ cm^{-1}. Ref: 307.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3Si^{28}H$	871	1, ← 0,	Ground						10 690.34	.10	307
		2, ← 1,	Ground						21 380.58	.10	307
		3, ← 2,	Excited						32 040.2	.2	134
		3, ← 2,	Excited						32 043.3	.3	134
		3, ← 2,	Ground						32 070.2	.1	134
		3, ← 2,	Excited						32 101.2	.1	134
		3, ← 2,	Excited						32 159.9	.2	134
		3, ← 2,	Excited						32 248.4	.2	134
$(C^{12}H_3)_3Si^{28}D$	872	1, ← 0,	Ground						10 319.4	.10	307
		2, ← 1,	Ground						20 638.87	.10	307
		3, ← 2,	Excited						30 928.5	.1	134
		3, ← 2,	Excited						30 933.4	.2	134
		3, ← 2,	Ground						30 957.8	.1	134
		3, ← 2,	Excited						30 982.0	.2	134
		3, ← 2,	Excited						31 047.5	.2	134
$(C^{12}H_3)_3Si^{29}H$	873	2, ← 1,	Ground						21 351.36	.20	307
		3, ← 2,	Ground						32 026.1	.2	134
$(C^{12}H_3)_3Si^{29}D$	874	2, ← 1,	Ground						20 615.49	.20	307
		3, ← 2,	Ground						30 916.4	.1	134
$(C^{12}H_3)_3Si^{30}H$	875	2, ← 1,	Ground						21 323.35	.20	307
		3, ← 2,	Ground						31 984.1	.3	134
$(C^{12}H_3)_3Si^{30}D$	876	2, ← 1,	Ground						20 592.50	.20	307
		3, ← 2,	Ground						30 875.6	.2	134
$C^{13}H_3(C^{12}H_3)_2Si^bH$	877	1, 1, 0← 0, 0, 0	Ground						10 514.75	.1	307
		2, 1, 1← 1, 0, 1	Ground						20 860.02	.1	307
		2, 2, 0← 1, 1, 0	Ground						21 039.24	.1	307
		2, 2, 1← 1, 1, 1	Ground						21 199.01	.1	307
$(C^{13}H_3)_2C^{12}H_3Si^bH$	878	2, 1, 1← 1, 0, 1	Ground						20 512.02	.1	307
		2, 2, 0← 1, 1, 0	Ground						20 690.03	.1	307
		2, 2, 1← 1, 1, 1	Ground						20 848.06	.1	307
$(C^{12}D_3)_2C^{12}H_3Si^bH$	879	1, 1, 0← 0, 0, 0	Ground						8 941.09	.1	307
		2, 1, 1← 1, 0, 1	Ground						17 346.60	.2	307
		2, 1, 1← 1, 0, 1	Ground						17 358.67	.2	307
		2, 1, 1← 1, 0, 1	Ground						17 374.08	.1	307
		2, 2, 0← 1, 1, 0	Ground						17 966.81	.2	307
		2, 2, 0← 1, 1, 0	Ground						17 974.66	.2	307
		2, 2, 0← 1, 1, 0	Ground						17 987.14	.1	307
		2, 2, 1← 1, 1, 1	Ground						18 372.55	.2	307
		2, 2, 1← 1, 1, 1	Ground						18 378.75	.2	307
		2, 2, 1← 1, 1, 1	Ground						18 390.30	.1	307
s-$C^{12}H_2D(C^{12}H_3)_2Si^bD$	881	2, 1, 1← 1, 0, 1	Ground						19 787.30	.10	307
		2, 2, 0← 1, 1, 0	Ground						19 962.62	.10	307
		2, 2, 1← 1, 1, 1	Ground						20 116.38	.10	307
a-$C^{12}H_2D(C^{12}H_3)_2Si^bD$	882	2, 1, 1← 1, 0, 1	Ground						19 736.85	.10	307
		2, 2, 0← 1, 1, 0	Ground						20 068.81	.10	307
		2, 2, 1← 1, 1, 1	Ground						20 333.25	.10	307
s-$C^{12}D_2H(C^{12}H_3)_2Si^bD$	883	2, 1, 1← 1, 0, 1	Ground						19 063.92	.10	307
		2, 2, 0← 1, 1, 0	Ground						19 544.30	.10	307
		2, 2, 1← 1, 1, 1	Ground						19 892.55	.10	307
a-$C^{12}D_2H(C^{12}H_3)_2Si^bD$	884	2, 1, 1← 1, 0, 1	Ground						19 002.95	.10	307
		2, 2, 0← 1, 1, 0	Ground						19 470.41	.10	307
		2, 2, 1← 1, 1, 1	Ground						19 808.32	.10	307

$C_4H_3F_3$ $C_{3v}(C_{3v},C_{3v})$ $CH_3C{:}CCF_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}{:}C^{12}C^{12}F_3^{19}$	C_{3v}	891		1 369.70 M	1 369.70 M		.001	.998	
$C^{12}D_3C^{12}{:}C^{12}C^{12}F_3^{19}$	C_{3v}	892		1 229.15 M	1 229.15 M				
$C^{13}H_3C^{12}{:}C^{12}C^{12}F_3^{19}$	C_{3v}	893		1 329.84 M	1 329.84 M				
$C^{12}H_3C^{13}{:}C^{12}C^{12}F_3^{19}$	C_{3v}	894		1 356.78 M	1 356.78 M				
$C^{12}D_3C^{13}{:}C^{12}C^{12}F_3^{19}$	C_{3v}	895		1 219.81 M	1 219.81 M				
$C^{12}D_3C^{12}{:}C^{12}C^{13}F_3^{19}$	C_{3v}	896		1 226.93 M	1 226.93 M				
$C^{12}D_2HC^{12}{:}C^{12}C^{12}F_3^{19}$	C_s	897		1 271.85 M	1 271.85 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
891					300						

References:

ABC: 162 D_J: D_{JK}: 112 κ: 162 Δ:

μ: eQq: V: 350 I: ω:

Add. Refs.: 65, 247

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{:}C^{12}C^{12}F_3^{19}$	891	7, ← 6,	Ground						19 176.2	.1	162
		7, ← 6,	Excited						19 214.8	.1	162
		7, ← 6,	Excited						19 252.4	.1	162
		7, ← 6,	Excited						19 291.0	.1	162
		7, ← 6,	Excited						19 328.	2.	162
		8, ← 7,	Ground						21 915.2	.1	162
		9, ← 8,	Ground						24 654.5	.1	162
		10, ← 9,	Ground						27 393.6	.1	162
$C^{12}D_3C^{12}{:}C^{12}C^{12}F_3^{19}$	892	8, ← 7,	Ground						19 666.3	.1	162
		10, ← 9,	Ground						24 582.8	.1	162
		11, ←10,	Ground						27 041.8	.1	162
$C^{13}H_3C^{12}{:}C^{12}C^{12}F_3^{19}$	893	7, ← 6,	Ground						18 617.5	.5	162
		8, ← 7,	Ground						21 278.0	.5	162
		9, ← 8,	Ground						23 937.0	.5	162
		10, ← 9,	Ground						26 596.5	.5	162
$C^{12}H_3C^{13}{:}C^{12}C^{12}F_3^{19}$	894	7, ← 6,	Ground						18 995.0	.5	162
		8, ← 7,	Ground						21 708.5	.5	162
		9, ← 8,	Ground						24 422.5	.5	162
		10, ← 9,	Ground						27 135.0	.5	162
$C^{12}D_3C^{13}{:}C^{12}C^{12}F_3^{19}$	895	8, ← 7,	Ground						19 516.0	.5	162
		10, ← 9,	Ground						24 397.0	.5	162
		11, ←10,	Ground						26 836.0	2.	162
$C^{12}D_3C^{12}{:}C^{12}C^{13}F_3^{19}$	896	8, ← 7,	Ground						19 631.0	.5	162
		10, ← 9,	Ground						24 539.0	.5	162
		11, ←10,	Ground						26 992.0	.5	162
$C^{12}D_2HC^{12}{:}C^{12}C^{12}F_3^{19}$	897	8, , ← 7, ,	Ground						20 349.5	.5	162
		9, , ← 8, ,	Ground						22 893.5	.1	162
		10, , ← 9, ,	Ground						25 436.8	.1	162
		11, , ←10, ,	Ground						27 980.8	.1	162

C_4H_5Cl $C_s(C_{3v},C_s)$ $CH_3C{:}CCH_2Cl$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}{:}C^{12}C^{12}H_2Cl^{35}$	C_s	901	17 631. M	1 490.55 M	1 385.06 M	0.40	−28.4		
$C^{12}H_3C^{12}{:}C^{12}C^{12}H_2Cl^{37}$	C_s	902	17 329. M	1 459.76 M	1 357.26 M	0.27	−21.6		

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
901	2.17 T		0. X		<100						

References:

ABC: 252 D_J: 252 D_{JK}: 252 κ: Δ:

μ: 380 eQq: V: 252 I: ω:

Add. Ref.: 221

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}:C^{12}C^{12}H_2Cl^{35}$	901	7, 0, 7← 6, 0, 6	Ground						20 100.		252
		7, 1, 6← 6, 1, 5	Ground						20 491.7	.15	252
		7, 1, 7← 6, 1, 6	Ground						19 753.23	.05	252
		7, 3, 4← 6, 3, 3	Ground						20 136.7	.15	252
		7, 3, 5← 6, 3, 4	Ground						20 136.7	.15	252
		7, 4, 3← 6, 4, 2	Ground						20 137.8	.15	252
		7, 4, 4← 6, 4, 3	Ground						20 137.8	.15	252
		8, 0, 8← 7, 0, 7	Ground						22 960.93	.05	252
		8, 1, 7← 7, 1, 6	Ground						23 416.04	.05	252
		8, 1, 8← 7, 1, 7	Ground						22 572.56	.05	252
		8, 2, 6← 7, 2, 5	Ground						23 042.71	.05	252
		8, 2, 7← 7, 2, 6	Ground						22 999.59	.05	252
		8, 3, 5← 7, 3, 4	Ground						23 014.4	.15	252
		8, 3, 6← 7, 3, 5	Ground						23 014.4	.15	252
		8, 4, 4← 7, 4, 3	Ground						23 014.4	.15	252
		8, 4, 5← 7, 4, 4	Ground						23 014.4	.15	252
		9, 0, 9← 8, 0, 8	Ground						25 817.70	.05	252
		9, 1, 8← 8, 1, 7	Ground						26 339.34	.05	252
		9, 1, 9← 8, 1, 8	Ground						25 390.67	.05	252
		9, 2, 7← 8, 2, 6	Ground						25 933.76	.05	252
		9, 2, 8← 8, 2, 7	Ground						25 872.05	.05	252
		9, 3, 6← 8, 3, 5	Ground						25 892.2	.15	252
		9, 3, 7← 8, 3, 6	Ground						25 892.2	.15	252
		9, 4, 5← 8, 4, 4	Ground						25 892.2	.15	252
		9, 4, 6← 8, 4, 5	Ground						25 892.2	.15	252
		10, 0,10← 9, 0, 9	Ground						28 669.96	.05	252
		10, 1, 9← 9, 1, 8	Ground						29 261.28	.05	252
		10, 1,10← 9, 1, 9	Ground						28 207.61	.05	252
		10, 2, 8← 9, 2, 7	Ground						28 828.23	.05	252
		10, 2, 9← 9, 2, 8	Ground						28 743.74	.05	252
		10, 3, 7← 9, 3, 6	Ground						28 772.3	.15	252
		10, 3, 8← 9, 3, 7	Ground						28 770.2	.15	252
		10, 4, 6← 9, 4, 5	Ground						28 770.2	.15	252
		10, 4, 7← 9, 4, 6	Ground						28 770.2	.15	252
$C^{12}H_3C^{12}:C^{12}C^{12}H_2Cl^{37}$	902	9, 0, 9← 8, 0, 8	Ground						25 293.3	.3	252
		9, 1, 9← 8, 1, 8	Ground						24 877.4	.3	252
		9, 3, 6← 8, 3, 5	Ground						25 363.7	.3	252
		9, 3, 7← 8, 3, 6	Ground						25 363.7	.3	252
		9, 4, 5← 8, 4, 4	Ground						25 363.7	.3	252
		9, 4, 6← 8, 4, 5	Ground						25 363.7	.3	252
		10, 0,10← 9, 0, 9	Ground						28 087.9	.3	252
		10, 1, 9← 9, 1, 8	Ground						28 661.5	.3	252
		10, 1,10← 9, 1, 9	Ground						27 637.7	.3	252
		10, 3, 7← 9, 3, 6	Ground						28 183.7	.3	252
		10, 3, 8← 9, 3, 7	Ground						28 183.7	.3	252
		10, 5, 5← 9, 5, 4	Ground						28 183.7	.3	252
		10, 5, 6← 9, 5, 5	Ground						28 183.7	.3	252
		11, 0,11←10, 0,10	Ground						30 877.9	.3	252

C_4H_5F $C_s(C_s,C_s,C_s)$ $CH_2{:}CHCF{:}CH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_2{:}C^{12}HC^{12}F^{19}{:}C^{12}H_2$	C_s	911	10 006.26 M	4 264.35 M	2 989.21 M			−.64	.049

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
911	0.288 M	1.388 M	0. X					280[1] 1			

References:

ABC: 385 D_J: D_{JK}: κ: 385 Δ: 385

μ: 385 eQq: V: I: ω: 385

1. This value was given by Lide for the lowest bending mode.

2-Fluoro-1,3-Butadiene

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2{:}C^{12}HC^{12}F^{19}{:}C^{12}H_2$	911	1, 1, 1← 0, 0, 0	Ground	A 0					12 995.53	.03	385
		2, 1, 2← 1, 0, 1	Ground	A 0					18 973.87	.03	385
		2, 2, 0← 1, 1, 1	Ground	A 0					34 472.81	.03	385
		2, 2, 1← 1, 1, 0	Ground	A 0					33 007.94	.03	385
		2, 1, 2← 2, 0, 2	Ground	A 0					8 481.94	.03	385
		2, 2, 1← 2, 1, 2	Ground	A 0					21 051.13	.03	385
		3, 1, 3← 2, 0, 2	Ground	A 3					24 301.42	.03	385
		3, 1, 3← 2, 0, 2	1	A 1					24 352.94	.03	385
		3, 1, 3← 2, 0, 2	Ground	A 1					24 358.82	.03	385
		3, 1, 3← 2, 0, 2	Ground	A 0					24 393.53	.03	385
		3, 2, 2← 3, 1, 3	Ground	A 0					23 074.5	.2	385
		4, 0, 4← 3, 1, 3	1	A 0					23 904.63	.03	385
		4, 0, 4← 3, 1, 3	Ground	A 0					23 959.42	.03	385
		4, 0, 4← 3, 1, 3	1	A 1					23 962.2	.2	385
		4, 0, 4← 3, 1, 3	Ground	A 1					24 007.74	.03	385
		4, 0, 4← 3, 1, 3	Ground	A 2					24 051.09	.03	385
		4, 0, 4← 3, 1, 3	Ground	A 3					24 089.49	.03	385
		4, 1, 3← 4, 0, 4	Ground	A 0					14 799.7	.2	385
		4, 2, 3← 4, 1, 4	Ground	A 0					25 807.92	.03	385
		5, 0, 5← 4, 1, 4	1	A 0					31 080.55	.03	385
		5, 0, 5← 4, 1, 4	1	A 1					31 134.21	.03	385
		5, 0, 5← 4, 1, 4	Ground	A 0					31 140.55	.03	385
		5, 0, 5← 4, 1, 4	Ground	A 1					31 185.84	.03	385
		5, 0, 5← 4, 1, 4	Ground	A 2					31 227.04	.03	385
		5, 0, 5← 4, 1, 4	Ground	A 3					31 263.84	.03	385

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_2$:$C^{12}HC^{12}F^{19}$:$C^{12}H_2$	911	5, 1, 5← 4, 0, 4	Ground	A	0					34 586.04	.03	385
		5, 1, 4← 4, 2, 3	Ground	A	0					25 249.7	.2	385
		5, 2, 3← 5, 1, 4	Ground	A	0					16 148.9	.2	385
		5, 2, 4← 5, 1, 5	Ground	A	0					29 240.6	.2	385
		5, 3, 2← 5, 2, 3	Ground	A	4					27 324.1	.2	385
		5, 3, 2← 5, 2, 3	Ground	A	2					27 766.71	.03	385
		5, 3, 2← 5, 2, 3	Ground	A	1					28 031.28	.03	385
		5, 3, 2← 5, 2, 3	1	A	1					28 155.63	.03	385
		5, 3, 2← 5, 2, 3	Ground	A	0					28 323.90	.03	385
		5, 3, 2← 5, 2, 3	1	A	0					28 501.20	.03	385
		6, 1, 5← 6, 0, 6	Ground	A	4					25 316.9	.2	385
		6, 1, 5← 6, 0, 6	Ground	A	3					25 492.18	.03	385
		6, 1, 5← 6, 0, 6	Ground	A	2					25 682.88	.03	385
		6, 1, 5← 6, 0, 6	Ground	A	1					25 882.63	.03	385
		6, 1, 5← 6, 0, 6	Ground	A	0					26 089.45	.03	385
		6, 1, 5← 6, 0, 6	1	A	0					26 231.29	.03	385
		6, 2, 4← 6, 1, 5	Ground	A	0					17 778.5	.2	385
		6, 3, 3← 6, 2, 4	Ground	A	0					26 386.24	.03	385
		7, 2, 5← 7, 1, 6	Ground	A	0					20 907.7	.2	385
		7, 3, 4← 7, 2, 5	Ground	A	4					23 853.8	.2	385
		7, 3, 4← 7, 2, 5	Ground	A	3					24 036.17	.03	385
		7, 3, 4← 7, 2, 5	Ground	A	2					24 243.23	.03	385
		7, 3, 4← 7, 2, 5	Ground	A	1					24 475.25	.03	385
		7, 3, 4← 7, 2, 5	1	A	1					24 583.80	.03	385
		7, 3, 4← 7, 2, 5	Ground	A	0					24 732.10	.03	385
		7, 3, 4← 7, 2, 5	1	A	0					24 887.38	.03	385
		8, 2, 6← 8, 1, 7	Ground	A	4					24 858.1	.2	385
		8, 2, 6← 8, 1, 7	Ground	A	3					25 027.10	.03	385
		8, 2, 6← 8, 1, 7	Ground	A	2					25 212.69	.03	385
		8, 2, 6← 8, 1, 7	Ground	A	1					25 406.25	.03	385
		8, 2, 6← 8, 1, 7	Ground	A	0					25 605.61	.03	385
		8, 2, 6← 8, 1, 7	1	A	0					25 743.60	.03	385
		8, 3, 5← 8, 2, 6	Ground	A	3					23 294.78	.03	385
		8, 3, 5← 8, 2, 6	Ground	A	2					23 491.24	.03	385
		8, 3, 5← 8, 2, 6	Ground	A	1					23 709.41	.03	385
		8, 3, 5← 8, 2, 6	1	A	1					23 814.66	.03	385
		8, 3, 5← 8, 2, 6	Ground	A	0					23 948.98	.03	385
		8, 3, 5← 8, 2, 6	1	A	0					24 096.12	.03	385
		9, 3, 6← 9, 2, 7	Ground	A	3					23 879.11	.03	385
		9, 3, 6← 9, 2, 7	Ground	A	2					24 072.85	.03	385
		9, 3, 6← 9, 2, 7	Ground	A	1					24 284.40	.03	385
		9, 3, 6← 9, 2, 7	1	A	1					24 392.35	.03	385
		9, 3, 6← 9, 2, 7	Ground	A	0					24 512.80	.03	385
		9, 3, 6← 9, 2, 7	1	A	0					24 657.75	.03	385
		10, 3, 7←10, 2, 8	Ground	A	4					25 909.1	.2	385
		10, 3, 7←10, 2, 8	Ground	A	3					26 091.38	.03	385
		10, 3, 7←10, 2, 8	Ground	A	2					26 293.23	.03	385
		10, 3, 7←10, 2, 8	Ground	A	1					26 508.54	.03	385
		10, 3, 7←10, 2, 8	1	A	1					26 626.69	.03	385
		10, 3, 7←10, 2, 8	Ground	A	0					26 735.76	.03	385
		10, 3, 7←10, 2, 8	1	A	0					26 886.28	.03	385
		11, 3, 8←11, 2, 9	Ground	A	0					30 754.10	.03	385

C_4H_5N $C_s(C_{3v},C_s)$ t–$CH_3CH{:}CHCN$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
t-$C^{12}H_3C^{12}H{:}C^{12}HC^{12}N^{14}$	C_s	921	38 200. M	2 297.05 M	2 195.22 M	.00034	−.0126		

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
921	4.5 T		0. X		>2100						

References:

ABC: 293 D_J: 293 D_{JK}: 293 κ: Δ:

μ: 293 eQq: V: 293 I: ω:

trans-Crotononitrile

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
t-$C^{12}H_3C^{12}H{:}C^{12}HC^{12}N^{14}$	921	3, 0, ← 2, 0,	Ground						13 475.89	.5	293
		3, 1, ← 2, 1,	Ground						13 324.45	.5	293
		3, 1, ← 2, 1,	Ground						13 629.06	.5	293
		3, 2, ← 2, 2,	Ground						13 477.2	.5	293
		4, 0, ← 3, 0,	Ground						17 966.75	.5	293
		4, 1, ← 3, 1,	Ground						17 765.04	.5	293
		4, 1, ← 3, 1,	Ground						18 172.15	.5	293
		4, 2, ← 3, 2,	Ground						17 970.0	.5	293
		4, 3, ← 3, 3,	Ground						17 970.0	.5	293
		5, 0, ← 4, 0,	Ground						22 456.90	.5	293
		5, 1, ← 4, 1,	Ground						22 205.78	.5	293
		5, 1, ← 4, 1,	Ground						22 714.99	.5	293
		5, 3, ← 4, 3,	Ground						22 463.68	.5	293
		5, 4, ← 4, 4,	Ground						22 463.68	.5	293
		6, 0, ← 5, 0,	Ground						26 945.74	.5	293
		6, 1, ← 5, 1,	Ground						26 646.22	.5	293
		6, 1, ← 5, 1,	Ground						27 257.39	.5	293
		6, 2, ← 5, 2,	Ground						26 953.3	.5	293
		6, 2, ← 5, 2,	Ground						26 961.1	.5	293
		6, 3, ← 5, 3,	Ground						26 956.48	.5	293
		6, 4, ← 5, 4,	Ground						26 956.48	.5	293
		6, 5, ← 5, 5,	Ground						26 957.60	.5	293
		8, 0, ← 7, 0,	Ground						35 919.24	.5	293
		8, 1, ← 7, 1,	Ground						35 526.03	.5	293
		8, 1, ← 7, 1,	Ground						36 340.65	.5	293
		8, 2, ← 7, 2,	Ground						25 954.3	.5	293
		8, 2, ← 7, 2,	Ground						35 936.2	.5	293
		8, 3, ← 7, 3,	Ground						35 942.6	.5	293
		8, 4, ← 7, 4,	Ground						35 942.6	.5	293
		8, 5, ← 7, 5,	Ground						35 943.5	.5	293
		8, 6, ← 7, 6,	Ground						35 945.6	.5	293
		8, 7, ← 7, 7,	Ground						35 948.4	.5	293

C_4H_6 $C_s(C_{3v},C_s)$ $CH_3CH{:}C{:}CH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}H{:}C^{12}{:}C^{12}H_2$	C_s	931	33 860. M	4 201.26 M	3 928.11 M	.0012	−.054		152.8

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
931	0.394 M	0.070 M	0. X		1589	6					

References:

ABC: 182 D_J: 182 D_{JK}: 182 κ: Δ: 182

μ: 182 eQq: V: 182 I: ω:

1,2-Butadiene

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}H{:}C^{12}{:}C^{12}H_2$	931	2, 0, 2← 1, 0, 1	Ground	E	0					16 256.76	.03	182
		2, 0, 2← 1, 0, 1	Ground	A	0					16 256.93	.03	182
		2, 1, 1← 1, 1, 0	Ground	E	0					16 529.90	.03	182
		2, 1, 1← 1, 1, 0	Ground	A	0					16 532.29	.03	182
		2, 1, 2← 1, 1, 1	Ground	A	0					15 985.82	.03	182
		2, 1, 2← 1, 1, 1	Ground	E	0					15 987.84	.03	182
		3, 0, 3← 2, 0, 2	Ground	E	0					24 380.36	.03	182
		3, 0, 3← 2, 0, 2	Ground	A	0					24 380.63	.03	182
		3, 1, 2← 2, 1, 1	Ground	E	0					24 796.20	.03	182
		3, 1, 2← 2, 1, 1	Ground	A	0					24 797.09	.03	182
		3, 1, 3← 2, 1, 2	Ground	A	0					23 977.46	.03	182
		3, 1, 3← 2, 1, 2	Ground	E	0					23 977.89	.03	182
		3, 2, 1← 2, 2, 0	Ground	E	0					24 393.2	.1	182
		3, 2, 1← 2, 2, 0	Ground	A	0					24 396.90	.03	182
		3, 2, 2← 2, 2, 1	Ground	A	0					24 389.35	.03	182
		3, 2, 2← 2, 2, 1	Ground	E	0					24 392.8	.03	182
		4, 0, 4← 3, 0, 3	Ground	E	0					32 498.28	.03	182
		4, 0, 4← 3, 0, 3	Ground	A	0					32 498.63	.03	182
		4, 1, 3← 3, 1, 2	Ground	E	0					33 059.64	.03	182
		4, 1, 3← 3, 1, 2	Ground	A	0					33 060.34	.03	182
		4, 1, 4← 3, 1, 3	Ground	A	0					31 967.61	.03	182
		4, 1, 4← 3, 1, 3	Ground	E	0					31 967.67	.03	182
		4, 2, 2← 3, 2, 1	Ground	E	0					32 528.1	.1	182
		4, 2, 2← 3, 2, 1	Ground	A	0					32 536.26	.03	182
		4, 2, 3← 3, 2, 2	Ground	A	0					32 517.58	.03	182
		4, 2, 3← 3, 2, 2	Ground	E	0					32 525.0	.1	182
		4, 3, 1← 3, 3, 0	Ground	E	0					32 525.0	.1	182
		4, 3, 1← 3, 3, 0	Ground	A	0					32 525.0	.1	182
		4, 3, 2← 3, 3, 1	Ground	E	0					32 525.0	.1	182
		4, 3, 2← 3, 3, 1	Ground	A	0					32 525.0	.1	182

C_4H_8 $C_{2v}(C_{3v},C_{3v},C_{2v})$ $(CH_3)_2C{:}CH_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_2C^{12}{:}C^{12}H_2$	C_{2v}	941	9 133.32 M	8 381.75 M	4 615.99 M				
a-$C^{12}H_2DC^{12}H_3C^{12}{:}C^{12}H_2$	C_1	942	8 819.46 M	7 981.08 M	4 469.59 M				
s-$C^{12}H_2DC^{12}H_3C^{12}{:}C^{12}H_2$	C_s	943	9 132.59 M	7 788.98 M	4 431.05 M				
$(C^{12}H_3)_2C^{12}{:}C^{12}HD$	C_1	944	8 693.49 M	8 114.67 M	4 422.67 M				
$C^{13}H_3C^{12}H_3C^{12}{:}C^{12}H_2$	C_1	945	9 074.31 M	8 149.00 M	4 529.72 M				
$(C^{12}H_3)_2C^{12}{:}C^{13}H_2$	C_2	946	8 810.08 M	8 381.73 M	4 531.84 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
941	0. X	0.503 M	0. X		2210						

References:

ABC: 326, 366 D_J: D_{JK}: κ: Δ:

μ: 326 eQq: V: 326 I: ω:

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_2C^{12}{:}C^{12}H_2$	941	2, 0, 2← 1, 1, 1	Ground							22 128.05	.05	326
		2, 1, 2← 1, 0, 1	Ground							22 981.28	.05	326
		2, 2, 1← 1, 1, 0	Ground							32 015.95	.05	326
		3, 0, 3← 2, 1, 2	Ground							31 768.96	.05	326
		3, 1, 3← 2, 0, 2	Ground							31 879.31	.05	326
		3, 1, 2← 3, 0, 3	Ground							20 279.79	.05	326
		3, 2, 2← 3, 1, 3	Ground							20 767.71	.05	326
		4, 1, 3← 4, 0, 4	Ground							28 771.06	.05	326
		4, 2, 2← 4, 1, 3	Ground							19 669.25	.05	326
		4, 2, 3← 4, 1, 4	Ground							28 830.61	.05	326
		4, 3, 2← 4, 2, 3	Ground							21 026.60	.05	326
		5, 2, 3← 5, 1, 4	Ground							28 557.28	.05	326
		5, 3, 2← 5, 2, 3	Ground							18 703.70	.05	326
		5, 4, 2← 5, 3, 3	Ground							21 519.40	.05	326
		5, 5, 1← 5, 4, 2	Ground							18 358.45	.05	326
		6, 3, 3← 6, 2, 4	Ground							28 121.48	.05	326
		6, 4, 3← 6, 3, 4	Ground							28 775.67	.05	326
		6, 5, 2← 6, 4, 3	Ground							22 320.86	.05	326
		6, 6, 1← 6, 5, 2	Ground							20 766.70	.05	326
		6, 6, 1← 6, 5, 2	Ground	E(−)	0					20 767.19		326
		6, 6, 1← 6, 5, 2	Ground	E(+)	0					20 767.23		326
		7, 5, 3← 7, 4, 4	Ground							28 851.31	.05	326
		7, 6, 2← 7, 5, 3	Ground							23 490.64	.05	326
		7, 7, 0← 7, 6, 1	Ground							19 736.70	.05	326
		7, 7, 0← 7, 6, 1	Ground	E(−)	0					19 737.40		326
		7, 7, 1← 7, 6, 2	Ground							23 524.94	.05	326
		7, 7, 1← 7, 6, 2	Ground	E	0					23 525.58		326
		8, 6, 3← 8, 5, 4	Ground							29 089.07	.05	326
		8, 8, 0← 8, 7, 1	Ground							23 994.84	.05	326
		8, 8, 0← 8, 7, 1	Ground	E(−)	0					23 995.50		326
		9, 6, 3← 9, 5, 4	Ground							24 638.80	.05	326
		9, 8, 1← 9, 7, 2	Ground							18 747.34	.05	326
		9, 8, 1← 9, 7, 2	Ground	E	0					18 748.06		326
		9, 9, 0← 9, 8, 1	Ground							28 220.48	.05	326
		9, 9, 0← 9, 8, 1	Ground	E(−)	0					28 221.17		326
		10, 7, 3←10, 6, 4	Ground							22 976.59	.05	326
		11, 9, 2←11, 8, 3	Ground							18 473.09	.05	326
		11, 9, 2←11, 8, 3	Ground	E(+)	0					18 473.73		326
		12,10, 2←12, 9, 3	Ground							21 449.36	.05	326
		12,10, 2←12, 9, 3	Ground	E(+)	0					21 450.11		326
		12,10, 2←12, 9, 3	Ground	E(−)	0					21 450.14		326
		14,12, 2←14,11, 3	Ground							29 909.89	.05	326
		14,12, 2←14,11, 3	Ground	E(+)	0					29 910.98		326
		14,12, 2←14,11, 3	Ground	E(−)	0					29 911.02		326
a-$C^{12}H_2DC^{12}H_3C^{12}{:}C^{12}H_2$	942	2, 0, 2← 1, 1, 1	Ground							21 256.85	.05	326
		2, 1, 2← 1, 0, 1	Ground							22 228.22	.05	326
		2, 2, 1← 1, 1, 0	Ground							30 927.96	.05	326
		3, 0, 3← 2, 1, 2	Ground							30 657.22	.05	326
		3, 1, 3← 2, 0, 2	Ground							30 803.61	.05	326
		3, 2, 2← 3, 1, 3	Ground							19 730.99	.05	326

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
a-$C^{12}H_2DC^{12}H_3C^{12}$:$C^{12}H_2$	942	4, 2, 2← 4, 1, 3	Ground						18 347.00	.05	326
		4, 3, 2← 4, 2, 3	Ground						20 065.05	.05	326
s-$C^{12}H_2DC^{12}H_3C^{12}$:$C^{12}H_2$	943	2, 0, 2← 1, 1, 1	Ground						20 752.87	.05	326
		2, 1, 2← 1, 0, 1	Ground						22 425.74	.05	326
		2, 2, 1← 1, 1, 0	Ground						31 828.82	.05	326
		3, 0, 3← 2, 1, 2	Ground						30 377.99	.05	326
		3, 1, 3← 2, 0, 2	Ground						30 759.55	.05	326
		3, 1, 2← 3, 0, 3	Ground						18 852.70	.05	326
		3, 2, 2← 3, 1, 3	Ground						20 334.26	.05	326
$(C^{12}H_3)_2C^{12}$:$C^{12}HD$	944	2, 0, 2← 1, 1, 1	Ground						21 319.80		366
		2, 1, 2← 1, 0, 1	Ground						21 961.51		366
		2, 2, 1← 1, 1, 0	Ground						30 503.15		366
		3, 0, 3← 2, 1, 2	Ground						30 475.68		366
		3, 1, 3← 2, 0, 2	Ground						30 542.80		366
		3, 1, 2← 3, 0, 3	Ground						19 639.41		366
		3, 1, 2← 3, 1, 3	Ground						19 944.54		366
$C^{13}H_3C^{12}H_3C^{12}$:$C^{12}H_2$	945	1, 1, 1← 0, 0, 0	Ground						13 604.08		366
		2, 0, 2← 1, 1, 1	Ground						21 582.34		366
		2, 1, 2← 1, 0, 1	Ground						22 663.50		366
		2, 2, 1← 1, 1, 0	Ground						31 752.65		366
		3, 0, 3← 2, 1, 2	Ground						31 153.16		366
		3, 1, 3← 2, 0, 2	Ground						31 325.69		366
		3, 1, 2← 3, 0, 3	Ground						19 764.88		366
		4, 2, 2← 4, 1, 3	Ground						18 905.09		366
		4, 3, 2← 4, 2, 3	Ground						20 889.82		366
$(C^{12}H_3)_2C^{12}$:$C^{13}H_2$	946	1, 1, 1← 0, 0, 0	Ground						13 342.01		366
		2, 0, 2← 1, 1, 1	Ground						21 943.47		366
		2, 1, 2← 1, 0, 1	Ground						22 405.60		366
		2, 2, 1← 1, 1, 0	Ground						30 962.08		366
		3, 0, 3← 2, 1, 2	Ground						31 233.01		366
		3, 1, 3← 2, 0, 2	Ground						31 268.52		366
		3, 1, 2← 3, 0, 3	Ground						20 174.97		366
		3, 2, 2← 3, 1, 3	Ground						20 340.93		366
		4, 2, 2← 4, 1, 3	Ground						19 947.74		366
		4, 3, 2← 4, 2, 3	Ground						20 429.62		366

C_4H_8O $C_s(C_{3v},C_s,C_{2v})$ $CH_3C^*H_2OC^*CH_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C^{12}H_3C^{12}{}_*H_2O^{16}C^{12}{}_*C^{12}H_3$	C_s	951	8 057.71 M	4 461.36 M	3 468.60 M			−.567	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
951	0. X	1.55 M	1.32 M		1607	150					

References:

ABC: 335 D_J: D_{JK}: κ: Δ:

μ: 335 eQq: V: 335 I: ω:

Coupling Parameter: $I_\alpha = 3.194$ amu Å2. Ref: 335.

cis-2,3-Epoxybutane Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C^{12}H_3C^{12}{}_*H_2O^{16}C^{12}{}_*C^{12}H_3$	951	1, 1, 1← 0, 0, 0	Ground						11 526.30	.2	335
		2, 1, 1← 1, 0, 1	Ground						21 441.30	.2	335
		2, 1, 2← 1, 0, 1	Ground						18 463.52	.2	335
		2, 2, 1← 1, 1, 1	Ground						28 634.49	.2	335
		2, 2, 0← 2, 1, 1	Ground						10 967.72	.2	335
		3, 0, 3← 2, 1, 2	Ground						20 327.53	.2	335
		3, 2, 1← 3, 1, 2	Ground						10 281.98	.2	335
		3, 2, 2← 3, 1, 2	Ground						9 423.92	.2	335
		4, 1, 3← 4, 0, 4	Ground						10 887.01	.2	335
		4, 2, 2← 4, 1, 3	Ground						10 099.17	.2	335
		4, 3, 2← 4, 2, 3	Ground						21 011.14	.2	335
		5, 2, 3← 5, 1, 4	Ground						10 771.40	.2	335
		7, 3, 5← 7, 2, 5	Ground						11 973.07	.2	335
		7, 3, 5← 7, 2, 6	Ground						24 993.89	.2	335
		8, 2, 6← 8, 1, 7	Ground	EE 0					19 666.15	.2	335
		8, 2, 6← 8, 1, 7	Ground	AE 0					19 667.05	.2	335
		8, 2, 6← 8, 1, 7	Ground	AA 0					19 667.94	.2	335
		8, 3, 6← 8, 2, 6	Ground						9 168.84	.2	335
		8, 4, 4← 8, 3, 5	Ground						23 798.49	.2	335
		10, 4, 6←10, 3, 7	Ground						20 556.93	.2	335
		11, 4, 7←11, 3, 8	Ground						20 201.05	.2	335
		16, 6,11←16, 5,11	Ground	AE 0					26 072.78	.2	335
		17, 6,12←17, 5,12	Ground	AA 0					20 888.81	.2	335
		17, 6,12←17, 5,12	Ground	AE 0					20 889.68	.2	335
		17, 6,12←17, 5,12	Ground	EE 0					20 890.57	.2	335
		19, 6,14←19, 5,14	Ground	AA 0					11 204.67	.2	335
		19, 6,14←19, 5,14	Ground	AE 0					11 205.59	.2	335
		19, 6,14←19, 5,14	Ground	EE 0					11 206.47	.2	335
		23, 7,17←23, 6,17	Ground	AA 0					9 641.95	.2	335
		23, 7,17←23, 6,17	Ground	AE 0					9 643.07	.2	335
		23, 7,17←23, 6,17	Ground	EE 0					9 644.25	.2	335

C_4H_9Br $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CBr$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}Br^{79}$	C_{3v}	961		2 044.2 M	2 044.2 M				
$(C^{12}H_3)_3C^{12}Br^{81}$	C_{3v}	962		2 028.3 M	2 028.3 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
961	2.21 M	0. X	0. X	511.6							
962				427.4							

References:

ABC: 339 D_J: D_{JK}: κ: Δ:

μ: 339 eQq: 339 V: I: ω:

Add. Ref.: 33

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}Br^{79}$	961	5, ← 4,	Ground						20 441.9	.3	134
		5, 0← 4, 0	Ground			11/2		9/2	20 439.6	.5	339[1]
		5, 0← 4, 0	Ground			13/2		11/2	20 439.6	.5	339[1]
		5, 0← 4, 0	Ground			7/2		5/2	20 448.1	.5	339[1]
		5, 0← 4, 0	Ground			9/2		7/2	20 449.6	.5	339
		5, 1← 4, 1	Ground			13/2		11/2	20 437.6	.5	339
		5, 1← 4, 1	Ground			7/2		5/2	20 443.3	.5	339
		5, 1← 4, 1	Ground			11/2		9/2	20 443.7	.5	339
		5, 1← 4, 1	Ground			9/2		7/2	20 448.1	.5	339[1]
		5, 2← 4, 2	Ground			7/2		5/2	20 427.3	.5	339
		5, 2← 4, 2	Ground			13/2		11/2	20 431.7	.5	339
		5, 2← 4, 2	Ground			9/2		7/2	20 453.3	.5	339
		5, 2← 4, 2	Ground			11/2		9/2	20 456.8	.5	339
		5, 3← 4, 3	Ground			7/2		5/2	20 400.9	.5	339
		5, 3← 4, 3	Ground			13/2		11/2	20 421.0	.5	339
		5, 3← 4, 3	Ground			9/2		7/2	20 459.7	.5	339
		5, 3← 4, 3	Ground			11/2		9/2	20 479.0	.5	339
		5, 4← 4, 4	Ground			7/2		5/2	20 365.3	.5	339
		5, 4← 4, 4	Ground			13/2		11/2	20 406.5	.5	339
		5, 4← 4, 4	Ground			9/2		7/2	20 468.0	.5	339
		5, 4← 4, 4	Ground			11/2		9/2	20 509.3	.5	339
		6, ← 5,	Ground						24 538.1	.3	134
		7, ← 6,	Ground						28 622.2	.3	134
		8, ← 7,	Ground						32 720.8	.3	134
		9, ← 8,	Ground						36 809.8	.3	134
		10, ← 9,	Ground						40 831.8	.3	134
$(C^{12}H_3)_3C^{12}Br^{81}$	962	5, 0← 4, 0	Ground			11/2		9/2	20 281.2	.5	339[1]
		5, 0← 4, 0	Ground			13/2		11/2	20 281.2	.5	339[1]
		5, 0← 4, 0	Ground			7/2		5/2	20 288.9	.5	339[1]
		5, 0← 4, 0	Ground			9/2		7/2	20 288.9	.5	339[1]
		5, 1← 4, 1	Ground			13/2		11/2	20 279.5	.5	339
		5, 1← 4, 1	Ground			11/2		9/2	20 284.7	.5	339
		5, 1← 4, 1	Ground			9/2		7/2	20 289.6	.5	339
		5, 2← 4, 2	Ground			7/2		5/2	20 271.3	.5	339
		5, 2← 4, 2	Ground			13/2		11/2	20 274.4	.5	339
		5, 2← 4, 2	Ground			9/2		7/2	20 293.2	.5	339
		5, 2← 4, 2	Ground			11/2		9/2	20 295.6	.5	339
		5, 3← 4, 3	Ground			7/2		5/2	20 249.8	.5	339
		5, 3← 4, 3	Ground			13/2		11/2	20 265.9	.5	339
		5, 3← 4, 3	Ground			9/2		7/2	20 297.8	.5	339
		5, 3← 4, 3	Ground			11/2		9/2	20 313.8	.5	339
		5, 4← 4, 4	Ground			7/2		5/2	20 219.7	.5	339
		5, 4← 4, 4	Ground			13/2		11/2	20 253.5	.5	339
		5, 4← 4, 4	Ground			9/2		7/2	20 304.6	.5	339
		5, 4← 4, 4	Ground			11/2		9/2	20 339.4	.5	339
		6, ← 5,	Ground						24 346.4	.3	134
		7, ← 6,	Ground						28 405.8	.3	134
		8, ← 7,	Ground						32 464.8	.3	134
		9, ← 8,	Ground						36 521.8	.3	134
		10, ← 9,	Ground						40 565.0	.3	134

1. There is a slight uncertainty as to which identification corresponds to which frequency for the $5_0 \leftarrow 4_0$ and $5_1 \leftarrow 4_1$ transitions in the $(CH_3)_3CBr^{79}$ species of Table I, reference 339. It is assumed that the assignment shown is correct.

C_4H_9Cl $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CCl$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}Cl^{35}$	C_{3v}	971		3 017.69 M	3 017.69 M				
$(C^{12}H_3)_3C^{12}Cl^{37}$	C_{3v}	972		2 953.54 M	2 953.54 M				
$(C^{12}H_3)_3C^{13}Cl^{35}$	C_{3v}	973		3 014.25 M	3 014.25 M				
$(C^{12}H_3)_3C^{13}Cl^{37}$	C_{3v}	974		2 949.79 M	2 949.79 M				
$C^{13}H_3(C^{12}H_3)_2C^{12}Cl^{35}$	C_s	975	4 460. M	3 002.36 M	2 965.87 M				
$(C^{12}D_3)_3C^{12}Cl^{35}$	C_{3v}	976		2 552.52 M	2 552.52 M				
$(C^{12}D_3)_3C^{12}Cl^{37}$	C_{3v}	977		2 500.22 M	2 500.22 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
971	2.13 M	0. X	0. X	−66.9							

References:

ABC: 340, 363 D_J: D_{JK}: κ: Δ:

μ: 363 eQq: 363 V: I: ω:

Add. Ref.: 359

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}Cl^{35}$	971	3, ← 2,	Ground						18 106.35	.10	363
		3, 0← 2, 0	Ground			3/2		1/2	18 102.76	.1	359
		3, 0← 2, 0	Ground			5/2		3/2	18 102.76	.1	359
		3, 0← 2, 0	Ground			7/2		5/2	18 107.19	.15	363
		3, 0← 2, 0	Ground			9/2		7/2	18 107.19	.15	363
		3, 1← 2, 1	Ground			7/2		7/2	18 095.24	.1	359
		3, 1← 2, 1	Ground			5/2		3/2	18 103.84	.15	363
		3, 1← 2, 1	Ground			7/2		5/2	18 103.84	.15	363
		3, 1← 2, 1	Ground			3/2		1/2	18 108.06	.15	363
		3, 1← 2, 1	Ground			9/2		7/2	18 108.06	.15	363
		3, 1← 2, 1	Ground			5/2		5/2	18 109.66	.1	359
		3, 1← 2, 1	Ground			3/2		3/2	18 116.23	.1	359
		3, 2← 2, 2	Ground			7/2		5/2	18 094.42	.15	363
		3, 2← 2, 2	Ground			5/2		5/2	18 094.42	.15	363
		3, 2← 2, 2	Ground			3/2		3/2	18 106.19	.1	359
		3, 2← 2, 2	Ground			5/2		3/2	18 106.19	.1	359
		3, 2← 2, 2	Ground			7/2		7/2	18 111.15	.15	363
		3, 2← 2, 2	Ground			9/2		7/2	18 111.15	.15	363
		3, 2← 2, 2	Ground			3/2		1/2	18 122.08	.1	359
		4, ← 3,	Ground						24 141.5	.10	134
		5, ← 4,	Ground						30 176.8	.10	363
		6, ← 5,	Ground						36 212.3	.10	363
		7, ← 6,	Ground						42 243.8	.3	134
$(C^{12}H_3)_3C^{12}Cl^{37}$	972	4, ← 3,	Ground						23 627.3	.3	134
		5, ← 4,	Ground						29 535.6	.3	363
		6, ← 5,	Ground						35 442.3	.3	363
		7, ← 6,	Ground						41 330.	30.	33
$(C^{12}H_3)_3C^{13}Cl^{35}$	973	5, ← 4,	Ground						30 142.5		363
		6, ← 5,	Ground						36 171.1		363
$(C^{12}H_3)_3C^{13}Cl^{37}$	974	5, ← 4,	Ground						29 498.0		363
		6, ← 5,	Ground						35 397.3		363
$C^{13}H_3(C^{12}H_3)_2C^{12}Cl^{35}$	975	5, 0, 5← 4, 0, 4	Ground						29 827.79	.20	363
		5, 1, 4← 4, 1, 3	Ground						29 929.33	.20	363
		5, 1, 5← 4, 1, 4	Ground						29 747.06	.20	363
		6, 0, 6← 5, 0, 5	Ground						35 785.80	.20	363
		6, 1, 5← 5, 1, 4	Ground						35 913.15	.20	363
		6, 1, 6← 5, 1, 5	Ground						35 694.66	.20	363
$(C^{12}D_3)_3C^{12}Cl^{35}$	976	4, ← 3,	Ground						20 417.9	3.	340
		5, ← 4,	Ground						25 528.0	3.	340
$(C^{12}D_3)_3C^{12}Cl^{37}$	977	4, ← 3,	Ground						20 001.5	3.	340
		5, ← 4,	Ground						25 002.5	3.	340

C_4H_9F $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CF$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}F^{19}$	C_{3v}	981	4 712.15 M	4 712.15 M		.0018			
$C^{13}H_3(C^{12}H_3)_2C^{12}F^{19}$	C_s	982	4 704.34 M	4 610.46 M	4 431.26 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
981	0. X	0. X	1.959 M		4300			428 1	493 2		
982	0. u	0. X	1.959 M								

References:

ABC: 226 D_J: 226 D_{JK}: κ: Δ:

μ: 226 eQq: V: 226 I: ω: 226

Add. Refs.: 63, 64

Rotational constants (B_v) for various vibrational modes:τ_a: 4709.04 MHz; τ_e: 4708.78 MHz; δ_a:4720.52 MHz; δ_e: 4713.73 MHz; ρ_e: 4704.10 MHz. Torsional frequencies: τ_a:223 ± 25 cm^{-1}. Ref: 226. Extra Reference: 184.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a ; v_b	Int. Rotor State	n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}F^{19}$	981	1, 0← 0, 0	Excited							9 408.0		226
		1, 0← 0, 0	Ground	E	1					9 417.7		226
		1, 0← 0, 0	Ground	A	1					9 418.0		226
		1, 0← 0, 0	Ground							9 424.30		226
		1, 0← 0, 0	0; 1							9 427.3		226
		1, 0← 0, 0	1; 0							9 441.0		226
		2, ← 1,	Excited							18 815.92		226
		2, ← 1,		E	3					18 817.5		63
		2, ← 1,		E	2					18 825.3		63
		2, ← 1,	Ground	A	1					18 836.09	.03	226
		2, ← 1,		E	1					18 836.3		63
		2, ← 1,	Ground							18 848.53	.03	226
		2, ← 1,		E	0					18 849.8		63
		2, ← 1,	1; 0							18 854.9		226
		2, ← 1,	0; 1							18 882.01		226
		2, 0← 1, 0		E	1					18 834.50		226[1]
		2, 1← 1, 1		E	1					18 821.63		226[1]
		2, 1← 1, 1		E	1					18 835.3		226[1]
		3, ← 2,	Excited							28 224.5		226
		3, ← 2,	Ground	A	1					28 254.05	.03	226
		3, ← 2,	Ground							28 272.72	.03	226
		3, ← 2,	1; 0							28 282.19		226
		3, ← 2,	0; 1							28 323.09		226
		3, 0← 2, 0		E	1					28 250.32		226[1]
		3, 1← 2, 1		E	1					28 232.47		226[1]
		3, 1← 2, 1		E	1					28 251.82		226[1]
		3, 2← 2, 2		E	1					28 252.49		226[1]
		3, 2← 2, 2		E	1					28 254.8		226[1]
$C^{13}H_3(C^{12}H_3)_2C^{12}F^{19}$	982	2, 1, 1← 1, 0, 1	Ground							18 536.		226
		2, 2, 0← 1, 1, 0	Ground							18 658.		226
		2, 2, 1← 1, 1, 1	Ground							18 723.		226
		3, 1, 2← 2, 0, 2	Ground							27 844.69	.03	226
		3, 2, 1← 2, 1, 1	Ground							27 824.92	.03	226
		3, 2, 2← 2, 1, 2	Ground							27 944.38	.03	226
		3, 3, 0← 2, 2, 0	Ground							28 044.08	.03	226
		3, 3, 1← 2, 2, 1	Ground							28 100.92	.03	226

1. *l*-doubling occurs here in the singly excited torsional state. A simple treatment of this is given in the reference by Lide and Mann.

C_4H_9I $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CI$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}I^{127}$	C_{3v}	991		1 562. M	1 562. M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
991	2.13 M	0. X	0. X								

References:

ABC: 33 D_J: D_{JK}: κ: Δ:

μ: 388 eQq: V: I: ω:

Add. Ref.: 389

2-Iodo-2-Methylpropane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}I^{127}$	991	9, ← 8,	Ground						28 085.	30.	33
		10, ← 9,	Ground						31 185.	30.	33
		11, ←10,	Ground						34 310.	30.	33
		12, ←11,	Ground						37 490.	30.	33
		13, ←12,	Ground						40 570.	30.	33

C_4H_{10} $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CH$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}H$	C_{3v}	1001	7 789.45 M	7 789.45 M		.011			
$(C^{12}H_3)_3C^{13}H$	C_{3v}	1002	7 773.88 M	7 773.88 M					
$(C^{12}H_3)_3C^{12}D$	C_{3v}	1003	7 540.82 M	7 540.82 M					
$(C^{13}H_3)(C^{12}H_3)_2C^{12}H$	C_s	1004	7 788.28 M	7 546.10 M	4 431. M				
s-$(C^{12}H_2D)(C^{12}H_3)_2C^{12}H$	C_s	1005	7 629.15 M	7 378.95 M	4 466. M				
a-$(C^{12}H_2D)(C^{12}H_3)_2C^{12}H$	C_1	1006	7 782.70 M	7 259.37 M	4 319. M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1001	0. X	0. X	0.132 M		3900			426 1	365 2		
1003	0. X	0. X	0.141 M								

References:

ABC: 266, 297 D_J: 297 D_{JK}: κ: Δ:

μ: 266, 297 eQq: V: 226 I: ω: 266

Add. Ref.: 146

Rotational constants (B_v) for various excited vibrational modes: τ_a: 7782.84 MHz; τ_e: 7774.67 MHz; δ_a: 7790.3 MHz; δ_e: 7795.0 MHz. Torsional frequencies: τ_a: 225 ± 20 cm^{-1}; τ_e: 280 ± 20 cm^{-1}. Ref: 226.

2-Methylpropane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a ; v_b	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}H$	1001	1, ← 0,	Ground	A 0					15 578.9		226
		2, ← 1,	Ground	E 1					31 098.35	.03	226
		2, ← 1,	Ground	A 1					31 130.99	.03	226
		2, ← 1,	Ground	A 0					31 157.46	.03	297
		2, ← 1,	1; 0	A 0					31 161.		226
		2, ← 1,	0; 1	A 0					31 180.		226
$(C^{12}H_3)_3C^{13}H$	1002	2, ← 1,		A 0					31 095.18	.10	297
$(C^{12}H_3)_3C^{12}D$	1003	2, ← 1,		A 0					30 162.95	.05	297
$(C^{13}H_3)(C^{12}H_3)_2C^{12}H$	1004	2, 1, 1← 1, 0, 1		A 0					30 426.24	.10	297
		2, 2, 0← 1, 1, 0		A 0					30 682.00	.10	297
		2, 2, 1← 1, 1, 1		A 0					30 910.58	.10	297
s-$(C^{12}H_2D)(C^{12}H_3)_2C^{12}H$	1005	2, 1, 1← 1, 0, 1		A 0					29 765.6	1.	297
		2, 2, 0← 1, 1, 0		A 0					30 031.28	.10	297
		2, 2, 1← 1, 1, 1		A 0					30 266.06	.20	297
a-$(C^{12}H_2D)(C^{12}H_3)_2C^{12}H$	1006	2, 1, 1← 1, 0, 1		A 0					29 560.45	.05	297
		2, 2, 0← 1, 1, 0		A 0					30 147.92	.05	297
		2, 2, 1← 1, 1, 1		A 0					30 607.11	.05	297

$C_4H_{10}O$ $C_{2v}(C_s,C_s)$ $C_2H_5OC_2H_5$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3C^{12}H_2)_2O^{16}$	C_{2v}	1011							

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1011		1.17 T									

References:

ABC: D_J: D_{JK}: κ: Δ:

μ: 372 eQq: V: I: ω:

Ethoxyethane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3C^{12}H_2)_2O^{16}$	1011	Not Reported							19 230.		396
		Not Reported							19 440.		396
		Not Reported							19 590.		396
		Not Reported							20 260.		396
		Not Reported							20 320.		396
		Not Reported							20 510.		396
		Not Reported							20 570.		396
		Not Reported							20 720.		396
		Not Reported							20 740.		396
		Not Reported							20 880.		396
		Not Reported							20 950.		396
		Not Reported							20 965.		396
		Not Reported							21 000.		396
		Not Reported							21 175.		396
		Not Reported							21 230.		396
		Not Reported							21 310.		396
		Not Reported							21 340.		396
		Not Reported							21 450.		396
		Not Reported							21 560.		396
		Not Reported							21 780.		396
		Not Reported							21 850.		396
		Not Reported							21 890.		396
		Not Reported							22 015.		396
		Not Reported							22 215.		396
		Not Reported							22 490.		396
		Not Reported							22 900.		396
		Not Reported							23 080.		396
		Not Reported							23 250.		396

C_5H_9N $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CCN$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}C^{12}N^{14}$	C_{3v}	1021		2 749.89 M	2 749.89 M				
$(C^{12}H_3)_3C^{12}C^{12}N^{15}$	C_{3v}	1022		2 676.87 M	2 676.87 M				
$(C^{13}H_3)(C^{12}H_3)_2C^{12}C^{12}N^{14}$	C_s	1023	4 513. M	2 738.45 M	2 707.87 M				
$(C^{12}H_3)_3C^{12}C^{13}N^{14}$	C_{3v}	1024		2 732.16 M	2 732.16 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1021	3.95 M	0. X	0. X		4000			183[1] 1			

1. Nugent, Mann and Lide state that evidence indicates that the frequency of the degenerate skeletal bending mode for tertiary-butyl cyanide is approximately the same as for tertiary-butyl acetylene.

References:

ABC: 353 D_J: D_{JK}: κ: Δ:

μ: 353 eQq: V: 353 I: ω: 353

Add. Ref.: 202

Rotational constants (B_v) for various excited vibrational modes: τ_a: 2748.84 MHz; τ_e: 2748.42 MHz; β_e: 2752.15 MHz. Ref: 353.

2,2-Dimethylpropanenitrile

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a^l	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}C^{12}N^{14}$	1021	4, 1← 3, 1	Ground						21 999.8	.2	190
		4, 2← 3, 2	Ground						21 999.8	.2	190
		4, 3← 3, 3	Ground						21 999.8	.2	190
		5, ← 4,	Ground	E 1					27 484.2	.1	353
		5, ← 4,	Ground	A 1					27 488.4	.1	353
		5, ← 4,	Ground						27 498.9	.1	353
		5, ← 4,	1, 0						27 521.5	.1	353
		5, 1← 4, 1	1,+1						27 539.1	.1	353[1]
		5, 1← 4, 1	Ground	E 1					27 474.9	.1	353[1]
$(C^{12}H_3)_3C^{12}C^{12}N^{15}$	1022	4, 1← 3, 1	Ground						21 414.8	.2	190
		4, 2← 3, 2	Ground						21 414.8	.2	190
		4, 3← 3, 3	Ground						21 414.8	.2	190
		5, ← 4,	Ground						26 768.7	.1	353
$(C^{13}H_3)(C^{12}H_3)_2C^{12}C^{12}N^{14}$	1023	5, 0, 5← 4, 0, 4	Ground						27 223.8	.1	353
		5, 1, 4← 4, 1, 3	Ground						27 306.5	.1	353
		5, 1, 5← 4, 1, 4	Ground						27 153.6	.1	353
		5, 2, 4← 4, 2, 3	Ground						27 238.6	.1	353
		4, 1, ← 3, 1,	Ground						21 850.	10.	190
		4, 2, ← 3, 2,	Ground						21 788.	2.	190
		4, 3, ← 3, 3,	Ground						21 788.	2.	190
$(C^{12}H_3)_3C^{12}C^{13}N^{14}$	1024	4, 1← 3, 1	Ground						21 850.	10.	190
		4, 2← 3, 2	Ground						21 850.	10.	190
		4, 3← 3, 3	Ground						21 850.	10.	190
		5, ← 4,	Ground						27 321.6	.1	353

1. Strong satellites of the J=5←4 line were assigned by Nugent, Mann and Lide to the lowest lying vibrational states, two of these lines to the degenerate skeletal bending mode which is the lowest lying Raman band. The weaker of these lines has been assigned to the l-type doublet $K=+1, l=+1$. l-type doubling also occurred for a line in the first excited torsional state, a similar pattern to that for the bending mode having been observed and assigned to $K=-1, l=-1$. The other components of the doublets were not resolved because of overlapping by unidentified vibrational satellites.

C_5H_9N $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CNC$

No molecular constant data

tert-Butyl Isocyanide

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}N^{14}C^{13}$	1031	4, ← 3,	Ground						22 786.5		203
$(C^{12}H_3)_3C^{12}N^{14}C^{12}$	1032	4, ← 3,	Ground						23 475.4		203

1040 - Nitrobenzene

Molecular Constant Table

$C_6H_5NO_2$ $C_{2v}(C_{2v},C_{2v})$ $C_6H_5NO_2$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C_6^{12}H_5N^{14}O_2^{16}$	C_{2v}	1041	4 011.7 M	1 283.8 M	974.3 M			−.7962	−.9

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1041	4.23 M	0. X	0. X								

References:

ABC: 309 D_J: D_{JK}: κ: 309 Δ: 309

μ: 309 eQq: V: I: ω:

Nitrobenzene

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C_6^{12}H_5N^{14}O_2^{16}$	1041	4, 0, 4← 3, 0, 3	Ground						8 793.	1.5	309
		4, 1, 3← 3, 1, 2	Ground						9 598.	1.5	309
		4, 2, 2← 3, 2, 1	Ground						9 251.	10.	309
		4, 2, 3← 3, 2, 2	Ground						9 013.	1.5	309
		4, 3, 1← 3, 3, 0	Ground						9 085.	2.5	309
		4, 3, 2← 3, 3, 1	Ground						9 085.	2.5	309
		8, 2, 7← 7, 2, 6	Ground						17 765.	2.	309
		8, 3, 6← 7, 3, 5	Ground						18 239.	6.	309
		8, 4, 5← 7, 4, 4	Ground						18 239.	6.	309
		8, 5, 4← 7, 5, 3	Ground						18 200.	4.	309
		8, 6, 2← 7, 6, 1	Ground						18 160.	5.	309
		8, 6, 3← 7, 6, 2	Ground						18 160.	5.	309
		8, 7, 2← 7, 7, 1	Ground						18 142.	4.	309
		8, 7, 3← 7, 7, 2	Ground						18 142.	4.	309
		9, 0, 9← 8, 0, 8	Ground						18 572.	2.	309
		10, 2, 8← 9, 2, 7	Ground						23 985.	3.	309
		10, 4, 6← 9, 4, 5	Ground						22 972.	3.	309
		10, 4, 7← 9, 4, 6	Ground						22 883.	3.	309

1050 - Phenol
Carbolic Acid; Hydroxybenzene

C_6H_6O C_s C_6H_5OH

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C_6^{12}H_5O^{16}H$	C_s	1051	5 650.46 M	2 619.20 M	1 789.84 M			−.5704	

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_2	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1051		1.45[1] T	0. X		1100	100.					

1. μ_a and μ_b would be expected to be roughly equal. Since only "b" type transitions have been observed and components of μ have not been resolved, the total dipole moment was entered as μ_b.

References:

ABC: 285 D_J: D_{JK}: κ: 285 Δ:

μ: 393 eQq: V: 285 I: ω:

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C_6^{12}H_5O^{16}H$	1051	4, 0, 4← 3, 1, 3	Ground						14 733.1		285[1]
		4, 0, 4← 3, 1, 3	Ground						14 844.9		285[1]
		4, 1, 4← 3, 0, 3	Ground						17 253.3		285[1]
		4, 1, 4← 3, 0, 3	Ground						17 365.1		285[1]
		5, 0, 5← 4, 1, 4	Ground						18 919.46		285[1]
		5, 0, 5← 4, 1, 4	Ground						19 031.50		285[1]
		5, 1, 5← 4, 0, 4	Ground						20 353.2		285[1]
		5, 1, 5← 4, 0, 4	Ground						20 465.3		285[1]
		5, 4, 1← 5, 3, 2	Ground						23 383.7		285[1]
		5, 4, 1← 5, 3, 2	Ground						23 494.8		285[1]
		5, 4, 2← 5, 3, 3	Ground						23 814.0		285[1]
		5, 4, 2← 5, 3, 3	Ground						23 925.5		285[1]
		6, 0, 6← 5, 1, 5	Ground						22 854.87		285[1]
		6, 0, 6← 5, 1, 5	Ground						22 967.07		285[1]
		6, 1, 6← 5, 0, 5	Ground						23 598.90		285[1]
		6, 1, 6← 5, 0, 5	Ground						23 710.65		285[1]
		6, 4, 2← 6, 3, 3	Ground						22 689.5		285[1]
		6, 4, 2← 6, 3, 3	Ground						22 800.6		285[1]
		6, 4, 3← 6, 3, 4	Ground						23 867.2		285[1]
		6, 4, 3← 6, 3, 4	Ground						23 978.6		285[1]
		7, 0, 7← 6, 1, 6	Ground						26 623.56		285[1]
		7, 0, 7← 6, 1, 6	Ground						26 735.31		285[1]
		7, 1, 7← 6, 1, 6	Ground						26 985.21		285[1]
		7, 1, 7← 6, 1, 6	Ground						27 097.02		285[1]
		7, 4, 3← 7, 3, 4	Ground						21 546.5		285[1]
		7, 4, 3← 7, 3, 4	Ground						21 658.1		285[1]
		7, 4, 4← 7, 3, 5	Ground						24 095.4		285[1]
		7, 4, 4← 7, 3, 5	Ground						24 206.8		285[1]
		8, 4, 4← 8, 3, 5	Ground						20 032.5		285[1]
		8, 4, 4← 8, 3, 5	Ground						20 145.3		285[1]
		8, 4, 5← 8, 3, 6	Ground						24 604.4		285[1]
		8, 4, 5← 8, 3, 6	Ground						24 715.9		285[1]
		9, 4, 5← 9, 3, 6	Ground						18 460.5		285[1]
		9, 4, 5← 9, 3, 6	Ground						18 572.1		285[1]
		9, 4, 6← 9, 3, 7	Ground						25 489.4		285[1]
		9, 4, 6← 9, 3, 7	Ground						25 601.4		285[1]
		10, 4, 6←10, 3, 7	Ground						17 284.4		285[1]
		10, 4, 6←10, 3, 7	Ground						17 396.2		285[1]
		10, 4, 7←10, 3, 8	Ground						26 821.7		285[1]
		10, 4, 7←10, 3, 8	Ground						26 932.8		285[1]
		11, 4, 7←11, 3, 8	Ground						16 945.3		285[1]
		11, 4, 7←11, 3, 8	Ground						17 056.8		285[1]
		11, 4, 8←11, 3, 9	Ground						28 629.7		285[1]
		11, 4, 8←11, 3, 9	Ground						28 741.2		285[1]
		12, 4, 8←12, 3, 9	Ground						17 752.3		285[1]
		12, 4, 8←12, 3, 9	Ground						17 864.0		285[1]

1. The splitting of each line in the spectrum is due to internal rotation of the OH group.

C_6H_9Cl $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CC{:}CCl$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{12}Cl^{35}$	C_{3v}	1061		891.69 M	891.69 M				
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{12}Cl^{37}$	C_{3v}	1062		868.24 M	868.24 M				

References:

ABC: 313 D_J: D_{JK}: κ: Δ:

μ: eQq: V: I: ω:

1-Chloro-3,3-Dimethyl-1-Butyne

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{12}Cl^{35}$	1061	11, ←10,	Ground						19 617.1	.5	313
		12, ←11,	Ground						21 400.5	.5	313
		13, ←12,	Ground						23 183.7	.5	313
		14, ←13,	Ground						24 967.1	.5	313
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{12}Cl^{37}$	1062	11, ←10,	Ground						19 101.2	.5	313
		12, ←11,	Ground						20 837.7	.5	313

C_6H_{10} $C_{3v}(C_{3v},C_{3v},C_{3v})$ $(CH_3)_3CC{:}CH$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{12}H$	C_{3v}	1071		2 683.18 M	2 683.18 M				
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{12}D$	C_{3v}	1072		2 531.09 M	2 531.09 M				
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{13}H$	C_{3v}	1073		2 609.35 M	2 609.35 M				
$(C^{12}H_3)_3C^{12}C^{13}{:}C^{12}H$	C_{3v}	1074		2 665.90 M	2 665.90 M				
$(C^{12}H_3)_3C^{12}C^{12}{:}C^{13}D$	C_{3v}	1075		2 467.53 M	2 467.53 M				
$(C^{12}H_3)_3C^{12}C^{13}{:}C^{12}D$	C_{3v}	1076		2 516.83 M	2 516.83 M				
$C^{13}H_3(C^{12}H_3)_2C^{12}C^{12}{:}C^{12}H$	C_s	1077		2 672.45 M	2 643.36 M				
$C^{13}H_3(C^{12}H_3)_2C^{12}C^{12}{:}C^{12}D$	C_s	1078		2 520.65 M	2 494.72 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V_3	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1071	0.661 M	0. X	0. X		4000			183 1			

References:

ABC: 313, 353 D_J: D_{JK}: κ: Δ:

μ: 353 eQq: V: 353 I: ω: 353

Rotational constants (B_v) for various excited vibrational modes: τ_a: 2682.05 MHz, τ_e: 2681.67 MHz, and β_e: 2685.77 MHz. Ref: 353.

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State v_a^l	Int. Rotor State n	Hyperfine F_t'	Hyperfine F'	Hyperfine F_t	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3C^{12}C^{12}:C^{12}H$	1071	2, ← 1,	Ground						10 732.9	.1	353
		3, ← 2,	Ground						16 099.3	.1	353
		4, ← 3,	Ground						21 453.5	.1	353
		4, ← 3,	Ground						21 456.4	.1	353
		4, ← 3,	Ground						21 465.5	.1	353
		4, ← 3,	1, 0						21 486.4	.1	353
		4, 1← 3, 1	1,+1						21 499.7	.1	353[1]
		4, 1← 3, 1	Ground						21 446.0	.1	353[1]
		5, ← 4,	Ground						26 816.8	.1	353
		5, ← 4,	Ground						26 820.4	.1	353
		5, ← 4,	Ground						26 831.9	.1	353
		5, ← 4,	1, 0						26 857.7	.1	353
		5, 1← 4, 1	1,+1						26 874.5	.1	353[1]
		5, 1← 4, 1	Ground						26 807.3	.1	353[1]
		6, ← 5,	Ground						32 179.8	.1	353
		6, ← 5,	Ground						32 184.3	.1	353
		6, ← 5,	1, 0						32 229.0	.1	353
		6, ← 5,	Ground						32 198.0	.1	353
		6, 1← 5, 1	1,+1						32 249.5	.1	353[1]
		6, 1← 5, 1	Ground						32 168.4	.1	353[1]
$(C^{12}H_3)_3C^{12}C^{12}:C^{12}D$	1072	4, ← 3,	Ground						20 248.8	.1	353
		5, ← 4,	Ground						25 310.9	.1	353
		6, ← 5,	Ground						30 373.0	.1	353
$(C^{12}H_3)_3C^{12}C^{12}:C^{13}H$	1073	4, ← 3,	Ground						20 874.9	.1	353
		5, ← 4,	Ground						26 093.5	.1	353
		6, ← 5,	Ground						31 312.1	.1	353
$(C^{12}H_3)_3C^{12}C^{13}:C^{12}H$	1074	4, ← 3,	Ground						21 327.2	.1	353
		5, ← 4,	Ground						26 659.1	.1	353
		6, ← 5,	Ground						31 990.5	.1	353
$(C^{12}H_3)_3C^{12}C^{12}:C^{13}D$	1075	4, ← 3,	Ground						19 740.3	.1	353
		5, ← 4,	Ground						24 675.4	.1	353
		6, ← 5,	Ground						29 610.2	.1	353
$(C^{12}H_3)_3C^{12}C^{13}:C^{12}D$	1076	4, ← 3,	Ground						20 134.6	.1	353
		5, ← 4,	Ground						25 168.2	.1	353
		6, ← 5,	Ground						30 201.9	.1	353
$C^{13}H_3(C^{12}H_3)_2C^{12}C^{12}:C^{12}H$	1077	4, 1, 3← 3, 1, 2	Ground						21 320.8	.1	353
		4, 1, 4← 3, 1, 3	Ground						21 204.4	.1	353
		5, 1, 4← 4, 1, 3	Ground						26 650.1	.1	353
		5, 1, 5← 4, 1, 4	Ground						26 504.7	.1	353
		6, 1, 5← 5, 1, 4	Ground						31 979.1	.1	353
		6, 1, 6← 5, 1, 5	Ground						31 804.5	.1	353
$C^{13}H_3(C^{12}H_3)_2C^{12}C^{12}:C^{12}D$	1078	4, 1, 3← 3, 1, 2	Ground						20 112.4	.1	353
		4, 1, 4← 3, 1, 3	Ground						20 009.0	.1	353
		5, 1, 4← 4, 1, 3	Ground						25 140.6	.1	353
		5, 1, 5← 4, 1, 4	Ground						25 010.9	.1	353
		6, 1, 5← 5, 1, 4	Ground						30 167.8	.1	353
		6, 1, 6← 5, 1, 5	Ground						30 012.2	.1	353

1. Strong satellites of the J = 4←3, 5←4, 6←5 lines were assigned by Nugent, Mann, and Lide to the lowest lying vibrational states, two of these being assigned to the degenerate skeletal bending mode which is the lowest Raman band, identified at 183 cm^{-1}. The weaker of these lines was assigned to the *l*-type doublet K = +1, *l* = +1. *l*-type doubling was also assigned for lines in the first excited torsional mode, a similar pattern to that for the bending mode having been observed. These were assigned to K = −1, *l* = −1. The other components of the doublets are not resolved because of overlapping by unidentified vibrational satellites.

$C_6H_{18}BN$ $C_{3v}(C_{3v},C_{3v},C_{3v},C_{3v},C_{3v},C_{3v})$ $(CH_3)_3N \cdot B(CH_3)_3$

Isotopic Species	Pt. Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$(C^{12}H_3)_3N^{14}\cdot B^{11}(C^{12}H_3)_3$	C_{3v}	1081		1 573.7 M	1 573.7 M				

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1081	3.92 L	0. X	0. X								

References:
ABC: 256 μ: 364

Add. Ref.: 301

Trimethylamine-Trimethylborane

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	F'	F_1	F	Frequency MHz	Acc. ±MHz	Ref.
$(C^{12}H_3)_3N^{14}\cdot B^{11}(C^{12}H_3)_3$	1081	6, ← 5,							18 884.	10.	256
		7, ← 6,							22 039.	10.	256
		8, ← 7,							25 179.	10.	256
		9, ← 8,							28 318.	10.	256

C_8H_6 $C_s(C_s,C_s)$ $C_6H_5C{:}CH$

Isotopic Species	Pt_1 Gp.	Id. No.	A (MHz)	B (MHz)	C (MHz)	D_J	D_{JK}	κ	Δ
$C_6^{12}H_5C^{12}{:}C^{12}H$	C_s	1091	5 662.86 M	1 530.09 M	1 204.38 M			−.8539	.80

Id. No.	μ_a Debye	μ_b Debye	μ_c Debye	eQq	V	Acc.	I_{red}	ω_a d	ω_b d	ω_c d	ω_d d
1091	0.78 T	0. X									

References:

ABC: 313 κ: 313 Δ: 338 μ: 395

Ethynylbenzene

Spectral Line Table

Isotopic Species	Id. No.	Rotational Quantum Nos.	Vib. State	Int. Rotor State n	Hyperfine F_1'	Hyperfine F'	Hyperfine F_1	Hyperfine F	Frequency MHz	Acc. ±MHz	Ref.
$C_6^{12}H_5C^{12}{:}C^{12}H$	1091	8, 3, 6← 7, 3, 5	Ground						22 023.6	.5	313
		8, 4, 4← 7, 4, 3	Ground						22 009.5	.5	313
		8, 4, 5← 7, 4, 4	Ground						22 003.4	.5	313
		8, 5, 3← 7, 5, 2	Ground						21 966.7	.5	313
		8, 5, 4← 7, 5, 3	Ground						21 966.7	.5	313
		8, 6, 2← 7, 6, 1	Ground						21 945.9	.5	313
		8, 6, 3← 7, 6, 2	Ground						21 945.9	.5	313
		8, 7, 1← 7, 7, 0	Ground						21 933.8	.5	313
		8, 7, 2← 7, 7, 1	Ground						21 933.8	.5	313
		9, 4, 5← 8, 4, 4	Ground						24 796.4	.5	313
		9, 5, 4← 8, 5, 3	Ground						24 732.1	.5	313
		9, 5, 5← 8, 5, 4	Ground						24 732.1	.5	313
		9, 6, 3← 8, 6, 2	Ground						24 702.7	.5	313
		9, 6, 4← 8, 6, 3	Ground						24 702.7	.5	313
		9, 7, 2← 8, 7, 1	Ground						24 685.6	.5	313
		9, 7, 3← 8, 7, 2	Ground						24 685.6	.5	313
		9, 8, 1← 8, 8, 0	Ground						24 674.5	.5	313
		9, 8, 2← 8, 8, 1	Ground						24 674.5	.5	313

5. Index According to Empirical Formula

Formula	Id. No.	Page
Inorganic		
F_2O_2	10	1
F_4N_2	20	3
HNO_3	30	4
H_2O_2	40	6
H_4N_2	50	10
Organic		
CF_8S	60	16
CH_2O_2	70	17
CH_3AsF_2	80	21
CH_3BF_2	90	31
CH_3Cl_3Ge	100	32
CH_3Cl_3Si	110	33
CH_3F_3Ge	120	34
CH_3F_3Si	130	34
CH_3NO	140	36
CH_3NO	150	40
CH_3NO_2	170	43
CH_3NO_3	180	49
CH_4F_2Si	190	51
CH_4O	210	56
CH_4S	220	65
CH_5ClSi	230	71
CH_5FSi	240	76
CH_5N	260	80
CH_5P	270	92
CH_6Ge	280	93
CH_6Si	310	97
CH_6Sn	340	100
C_2H_3BrO	350	101
C_2H_3ClO	360	106
$C_2H_3Cl_3$	380	118
C_2H_3FO	390	119
$C_2H_3F_3$	410	124
C_2H_3NS	420	126
C_2H_3NS	430	127
C_2H_4ClF	440	128
$C_2H_4Cl_2$	450	129
$C_2H_4F_2$	460	130
C_2H_4O	470	132
$C_2H_4O_2$	490	138
$C_2H_4O_2$	500	141
C_2H_5Br	520	145
C_2H_5Cl	540	151
C_2H_5F	550	158
C_2H_5I	570	162
C_2H_6O	580	165
C_2H_6O	590	166
Organic (continued)		
C_2H_6S	600	171
C_2H_6Si	610	177
C_2H_7N	630	180
C_2H_8Si	640	181
C_2H_8Si	650	184
$C_3H_3F_3O_4$	660	184
C_3H_3NO	670	185
C_3H_4O	680	190
C_3H_4O	690	191
C_3H_5F	700	192
C_3H_5F	710	194
C_3H_5F	720	196
C_3H_5N	730	199
C_3H_6	740	201
C_3H_6O	750	203
C_3H_6O	760	205
C_3H_7Cl	770	214
C_3H_8	780	216
C_3H_9As	790	218
$C_3H_9BF_3N$	800	219
C_3H_9BrSi	810	220
C_3H_9ClSi	820	221
C_3H_9FSi	830	222
C_3H_9ISi	840	223
C_3H_9N	850	224
C_3H_9P	860	225
$C_3H_{10}Si$	870	226
$C_4H_3F_3$	890	228
C_4H_5Cl	900	230
C_4H_5F	910	232
C_4H_5N	920	234
C_4H_6	930	235
C_4H_8	940	236
C_4H_8O	950	239
C_4H_9Br	960	240
C_4H_9Cl	970	242
C_4H_9F	980	244
C_4H_9I	990	246
C_4H_{10}	1000	247
$C_4H_{10}O$	1010	248
C_5H_9N	1020	249
C_5H_9N	1030	250
$C_6H_5NO_2$	1040	250
C_6H_6O	1050	251
C_6H_9Cl	1060	253
C_6H_{10}	1070	254
$C_6H_{18}BN$	1080	256
C_8H_6	1090	257

6. Index According to Chemical Name

Name	Id. No.	Page
A		
Acetaldehyde	470	132
Acetic Acid	490	138
Acetone	750	203
Acetyl Bromide	350	101
Acetyl Chloride	360	106
Acetyl Cyanide	670	185
Acetyl Fluoride	390	119
s-trans-Acrolein	690	191
Acrylaldehyde (see *s-trans*-Acrolein)	690	191
Acrylic Aldehyde (see *s-trans*-Acrolein)	690	191
Aminoethane (see Ethylamine)	630	180
Aminomethane (see Methylamine)	260	80
B		
Bromoethane	520	145
2-Bromo-2-methylpropane	960	240
1, 2-Butadiene	930	235
trans-2-Butenenitrile	920	234
C		
Carbolic Acid (see Phenol)	1050	251
1-Chloro-2-butyne	900	230
1-Chloro-3, 3-dimethyl-1-butyne	1060	253
Chloroethane	540	151
1-Chloro-2-fluoroethane	440	128
2-Chloro-2-methylpropane	970	242
Chloromethylsilane	230	71
Chloromethylsilicane (see Chloromethylsilane)	230	71
1-Chloropropane	770	214
trans-Crotonic Nitrile (see *trans*-Crotononitrile)	920	234
trans-Crotononitrile	920	234
D		
1, 2-Dichloroethane	450	129
Diethyl Ether	1010	248
1, 1-Difluoroethane	460	130
1, 1-Dimethyl-3-butyne	1070	254
Dimethyl Ether (see Methoxymethane)	590	166
α,α-Dimethylethyl Carbylamine (see *tert*-Butyl Isocyanide)	1030	250
Dimethyl Ketone (see Acetone)	750	203
Dimethylmethane (see Propane)	780	216
2, 2-Dimethylpropanenitrile	1020	249
α,α-Dimethylpropionitrile (see 2, 2-Dimethylpropanenitrile)	1020	249
Dioxygen Difluoride	10	1
Dimethylsilane	640	181
Dimethylsilicane (see Dimethylsilane)	640	181
Dimethyl Sulfide	600	171
E		
cis-2, 3-Epoxybutane	950	239
1, 2-Epoxypropane	760	205
Ethanal (see Acetaldehyde)	470	132
Ethanoic Acid (see Acetic Acid)	490	138
Ethanol	580	165
Ethanoyl Bromide (see Acetyl Bromide)	350	101
Ethanoyl Chloride (see Acetyl Chloride)	360	106
Ethanoyl Fluoride (see Acetyl Fluoride)	390	119
Ethenesilicane (see Vinyl Silane)	610	177
Ethoxyethane	1010	248
Ethyl Alcohol (see Ethanol)	580	165
Ethyl Bromide (see Bromoethane)	520	145
Ethyl Chloride (see Chloroethane)	540	151
Ethyl Cyanide (see Propionitrile)	730	199
Ethyl Fluoride (see Fluoroethane)	550	158
Ethyl Iodide (see Iodoethane)	570	162
Ethylamine	630	180
Ethylene Silane (see Vinyl Silane)	610	177
Ethylsilane	650	184
Ethylsilicane (see Ethylsilane)	650	184
Ethynylbenzene	1090	257
F		
2-Fluoro-1, 3-butadiene	910	232
Fluoroethane	550	158
2-Fluoro-2-methylpropane	980	244
Fluoroprene (see 2-Fluoro-1, 3-butadiene)	910	232
2-Fluoropropene	720	196
cis-1-Fluoropropene	700	192
trans-Fluoropropene	710	194
2-Fluoropropylene (see 2-Fluoropropene)	720	196
cis-α-Fluoropropylene (see *cis*-1-Fluoropropene)	700	192
trans-Fluoropropylene (see *trans*-Fluoropropene)	710	194
Formaldehyde Oxime (see Formaldoxime)	140	36
Formaldoxime	140	36
Formamide	150	40
Formic Acid	70	17
Formoxime (see Formaldoxime)	140	36
H		
Hydrazine	50	10
Hydrogen Peroxide	40	6
Hydroxybenzene (see Phenol)	1050	251
I		
Iodoethane	570	162
2-Iodo-2-methylpropane	990	246
Isobutane (see 2-Methylpropane)	1000	247
Isobutylene (see 2-Methylpropene)	940	236
Isopropenyl Fluoride (see 2-Fluoropropene)	720	196
M		
Methanamide (see Formamide)	150	40
Methanethiol	220	65
Methanoic Acid (see Formic Acid)	70	17
Methanol	210	56
Methoxymethane	590	166
Methyl Alcohol (see Methanol)	210	56
Methylallene (see 1, 2-Butadiene)	930	235
Methylamine	260	80
Methylchloroform (see 1, 1, 1-Trichloroethane)	380	118

6. Index According to Chemical Name (continued)

Name	Id. No.	Page
Methyldifluoroarsine	80	21
Methyldifluoroborane	90	31
Methyldifluorosilane	190	51
Methyldifluorosilicane (see Methyldifluorosilane)	190	51
Methyl Ethenone (see Methyl Ketene)	680	190
Methyl Ether (see Methoxymethane)	590	166
Methylethylene (see Propene)	740	201
Methyl Fluoroform (see 1, 1, 1-Trifluoroethane)	410	124
Methyl Formate	500	141
Methylgermane	280	93
Methyl Isothiocyanate	420	126
Methyl Ketene	680	190
Methyl Mercaptan (see Methanethiol)	220	65
Methyl Methanoate (see Methyl Formate)	500	141
Methylmonofluorosilane	240	76
Methylmonofluorosilicane (see Methylmonofluorosilane)	240	76
Methyl Nitrate	180	49
Methyloxirane (see 1, 2-Epoxypropane)	760	205
Methylphosphine	270	92
2-Methylpropane	1000	247
2-Methylpropene	940	236
Methylsilane	310	97
Methylsilicane (see Methylsilane)	310	97
Methylstannane	340	100
Methyl Nitrate	180	49
Methyl Sulfocyanate (see Methyl Thiocyanate)	430	127
Methyl Thiocyanate	430	127
Methylthiomethane (see Dimethyl Sulfide)	600	171
Methyltin (see Methylstannane)	340	100
Methyltrichlorogermane	100	32
Methyltrichlorosilane	110	33
Methyltrifluorogermane	120	34
Methyltrifluoromethylacetylene (see 1, 1, 1-Trifluoro-2-butyne)	890	228
Methyltrifluorosilane	130	34
Methyltrifluorosilicane (see methyltrifluorosilane)	130	34

N

Nitric Acid	30	4
Nitrobenzene	1040	250
Nitromethane	170	43

O

2-Oxopropanenitrile (see Pyruvonitrile)	670	185

P

Phenol	1050	251
Phenylacetylene (see Phenylethyne)	1090	257
Phenylethyne	1090	257
Propane	780	216
Propanenitrile (see Propionitrile)	730	199
2-Propanone (see Acetone)	750	203
Propenal (see *s-trans*-Acrolein)	690	191
Propene	740	201
Propene Oxide (see 1, 2-Epoxypropane)	760	205
trans-Propenyl Cyanide (see *trans*-2-Butenenitrile)	920	234
cis-Propenyl Fluoride (see *cis*-1-Fluoropropene)	700	192
trans-Propenyl Fluoride (see *trans*-Fluoropropene)	710	194
Propionitrile	730	199
n-Propyl Chloride (see 1-Chloropropane)	770	214
Propylene (see Propene)	740	201
Propylene Oxide (see 1,2-Epoxypropane)	760	205
Pyruvonitrile	670	185

T

tert-Butyl Acetylene (see 1, 1-Dimethyl-3-butyne)	1070	254
tert-Butyl Bromide (see 2-Bromo-2-methylpropane)	960	240
tert-Butyl Chloride (see 2-Chloro-2-methylpropane)	970	242
tert-Butyl Cyanide (see 2, 2-Dimethyl Propanenitrile)	1020	249
tert-Butyl Chloroacetylene (see 1-Chloro-3, 3-Dimethyl-1-Butyne)	1060	253
tert-Butyl Fluoride (see 2-Fluoro-2-methylpropane)	980	244
tert-Butyl Iodide (see 2-Iodo-2-methylpropane)	990	246
tert-Butyl Isocyanide	1030	250
Tetrafluorohydrazine	20	3
Tribromosilane	810	220
1, 1, 1-Trichloroethane	380	118
Trifluoroacetic Acid-Formic Acid Complex	660	184
Trifluoroborane-Trimethylamine	800	219
1, 1, 1-Trifluoro-2-butyne	890	228
1, 1, 1-Trifluoroethane	410	124
Trifluoromethyl Sulfur Pentafluoride	60	16
Trimethylacetonitrile (see 2, 2-Dimethyl Propionitrile)	1020	249
Trimethylamine	850	224
Trimethlyamine-trimethylborane	1080	256
Trimethylarsine	790	218
Trimethylbromoethane (see 2-Bromo-2-methylpropene)	960	240
Trimethylbromosilane	810	220
Trimethylbromosilicane	810	220
Trimethylchloromethane (see 2-Chloro-2-methylpropene)	970	242
Trimethylchlorosilane	820	221
Trimethylchlorosilicane (see Trimethylchlorosilane)	820	221
Trimethylfluoromethane (see 2-Fluoro-2-methylpropane)	980	244
Trimethylfluorosilane	830	222
Trimethylfluorosilicane (see Trimethylfluorosilane)	830	222
Trimethyliodomethane (see 2-Iodo-2-methylpropane)	990	246
Trimethyliodosilane	840	223
Trimethyliodosilicane (see Trimethyliodosilane)	840	223
Trimethylmethane (see 2-Methylpropane)	1000	247
Trimethylphosphine	860	225
Trimethylsilane	870	226
Trimethylsilicane (see Trimethylsilane)	870	226

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